

STIC Search Report Biotech-Chem Library

STIC Database Tracking Number: 149916

TO: Rei-Tsang Shiao Location: 5a10 / 5c18 Tuesday, April 12, 2005

Art Unit: 1626

Phone: 571-272-0707

Serial Number: 10 / 617431

From: Jan Delaval

Location: Biotech-Chem Library

Remsen 1a51

Phone: 571-272-22504

jan.delaval@uspto.gov

Search Notes			
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	Art Unit: 1026 P	hone Number of Date: [75] Date:
	Mail Box and Bldg/Room Le	Serial Number: $\frac{10}{611}$ $\frac{131}{131}$
		hone Number 50 2-070 / Serial Number: 10/6/12/13/ Results Format Preferred (circle): PAPER BISK E-MAIL
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	Please provide a detailed statement	of the search topic, and describe as specifically as possible the subject matter to be searched, tures, keywords, synonyms, acronyms, and registry numbers, and searched.
	nullity of the inventors 12 of	tures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or terms that may have a special meaning. Give examples or release
	known. Please attach a conv of the	tures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or terms that may have a special meaning. Give examples or relevant citations, authors, etc. if cover sheet, pertinent claims, and abstract.
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	Title of Invention:	lew fluorous tagging
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		nes): Zhang et al
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	Trespecte Serial number.	include all pertinent information (parent, child, divisional, or issued patent numbers) along with the
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=> fil reg FILE 'REGISTRY' ENTERED AT 07:12:31 ON 12 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 APR 2005 HIGHEST RN 848290-51-7 DICTIONARY FILE UPDATES: 11 APR 2005 HIGHEST RN 848290-51-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

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L26 ANSWER 1 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 649561-74-0 REGISTRY

ED Entered STN: 12 Feb 2004

CN Benzenesulfonamide, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H8 F17 N O2 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

$$\begin{array}{c|c} & \text{CH- (CF}_2)_{7} - \text{CF}_3 \\ & \\ \text{H}_2\text{N} - \\ & \\ \text{O} \end{array}$$

- **PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
 - 1 REFERENCES IN FILE CA (1907 TO DATE)
 - 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 2 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 649561-73-9 REGISTRY

ED Entered STN: 12 Feb 2004

CN Benzenesulfonamide, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H10 F17 N O2 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 649561-68-2 REGISTRY

ED Entered STN: 12 Feb 2004

CN 2H-Pyrimido[1,2-a]pyrimidine, 1-(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-

heptadecafluoroundecyl)-1,3,4,6,7,8-hexahydro- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H18 F17 N3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN **649561-67-1** REGISTRY

ED Entered STN: 12 Feb 2004

CN Benzene, 1-(chlorodiphenylmethyl)-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

MF C29 H18 C1 F17

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 649561-66-0 REGISTRY

ED Entered STN: 12 Feb 2004

CN Benzenemethanol, $4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-<math>\alpha,\alpha$ -diphenyl- (9CI) (CA INDEX NAME)

MF C29 H19 F17 O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 649561-59-1 REGISTRY

ED Entered STN: 12 Feb 2004

CN 2,5-Pyrrolidinedione, 1-[[[[2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-9H-fluoren-9-yl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C29 H18 F17 N O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN **649561-58-0** REGISTRY

ED Entered STN: 12 Feb 2004

CN 9H-Fluorene-9-methanol, 2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H15 F17 O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN **649561-57-9** REGISTRY

ED Entered STN: 12 Feb 2004

CN 9H-Fluorene, 2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H11 F17

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L26 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 556050-49-8 REGISTRY

ED Entered STN: 28 Jul 2003

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H14 F17 N O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:134436

REFERENCE 2: 140:128148

REFERENCE 3: 139:85611

L26 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN **544418-04-4** REGISTRY

ED Entered STN: 08 Jul 2003

CN 2H-3,1-Benzoxazine-2,4(1H)-dione, 1-(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,1

1-heptadecafluoroundecyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H10 F17 N O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 139:36318

L26 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN **514221-87-5** REGISTRY

ED Entered STN: 12 May 2003

CN 4-Piperidinecarboxylic acid, 1-(4-chlorobenzoyl)-, 4[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]phenyl
ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C29 H21 C1 F17 N O3 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

$$F_3C-(CF_2)_7-CH_2-CH_2-S$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:320984

L26 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 514221-86-4 REGISTRY

ED Entered STN: 12 May 2003

CN 4-Piperidinecarboxylic acid, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]phenyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H18 F17 N O2 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:320984

L26 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 514221-85-3 REGISTRY

ED Entered STN: 12 May 2003

CN 1,4-Piperidinedicarboxylic acid, 1-(1,1-dimethylethyl)
4-[4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]phen
yl] ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C27 H26 F17 N O4 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS, (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:320984

L26 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 501701-51-5 REGISTRY

ED Entered STN: 04 Apr 2003

CN Pyrimidine, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)sulfonyl]-6-methyl-2-[3-(trifluoromethyl)-1H-pyrazol1-yl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H10 F20 N4 O2 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

$$_{\text{F}_3\text{C}-\text{(CF}_2)}$$
 $_{7}-\text{CH}_2-\text{CH}_2-\text{S}$ $_{1}$ $_{0}$ $_{0}$ $_{1}$ $_{1}$ $_{0}$ $_{1}$ $_{1}$ $_{1}$ $_{1}$ $_{2}$ $_{3}$ $_{2}$ $_{3}$ $_{4}$ $_{2}$ $_{2}$ $_{3}$ $_{2}$ $_{3}$ $_{3}$ $_{4}$ $_{2}$ $_{3}$ $_{4}$ $_{2}$ $_{3}$ $_{4}$ $_{2}$ $_{3}$ $_{4}$ $_{5}$ $_{2}$ $_{3}$ $_{4}$ $_{5}$ $_{2}$ $_{3}$ $_{4}$ $_{5}$ $_{4}$ $_{5}$ $_{5}$ $_{5}$ $_{6}$ $_{7}$ $_{7}$ $_{1}$ $_{2}$ $_{3}$ $_{2}$ $_{3}$ $_{4}$ $_{2}$ $_{3}$ $_{4}$ $_{2}$ $_{3}$ $_{4}$ $_{4}$ $_{5}$ $_{5}$ $_{5}$ $_{5}$ $_{6}$ $_{7}$ $_{$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:238126

L26 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 501701-50-4 REGISTRY

ED Entered STN: 04 Apr 2003

CN Pyrimidine, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl)thio]-6-methyl-2-[3-(trifluoromethyl)-1H-pyrazol-1-

yl] - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H10 F20 N4 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

$$F_3C-(CF_2)_7-CH_2-CH_2-S$$

Me

N

N

CF₃

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:238126

L26 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 501701-48-0 REGISTRY

ED Entered STN: 04 Apr 2003

CN Pyrimidine, 2-chloro-4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-hontadegaflyaredegyl) thiel 6 methyl (001) (07 INDEX NAME)

heptadecafluorodecyl)thio]-6-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H8 Cl F17 N2 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:238126

L26 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 494798-73-1 REGISTRY

ED Entered STN: 25 Feb 2003

CN Benzaldehyde, 4-[(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-

heptadecafluoroundecyl)oxy] - (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[[3-(Perfluorooctyl)propyl]oxy]benzaldehyde

FS 3D CONCORD

MF C18 H11 F17 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:366039

REFERENCE 2: 140:128148

REFERENCE 3: 138:136691

L26 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 356055-77-1 REGISTRY

ED Entered STN: 12 Sep 2001

CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H11 F17 O

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, USPATFULL

$$CH_2-CH_2-(CF_2)_7-CF_3$$

 $HO-CH_2$

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 139:85611

REFERENCE 3: 135:256798

REFERENCE 4: 135:195695

L26 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 353525-52-7 REGISTRY

ED Entered STN: 29 Aug 2001

CN Benzene, 1-bromo-4-(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-

heptadecafluoroundecyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H10 Br F17

SR CA

LC STN Files: CA, CAPLUS, CASREACT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:166911

L26 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 340157-99-5 REGISTRY

ED Entered STN: 08 Jun 2001

CN Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-2-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H10 Br F17

SR CA

LC STN Files: CA, CAPLUS, CASREACT

$$CH_2-CH_2-(CF_2)_7-CF_3$$

Me

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:366630

L26 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 195324-88-0 REGISTRY

ED Entered STN: 14 Oct 1997

CN Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl) - (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)benzene

FS 3D CONCORD

MF C16 H8 Br F17

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:405395

REFERENCE 2: 140:128148

REFERENCE 3: 138:204515

REFERENCE 4: 137:262818

REFERENCE 5: 135:256798

REFERENCE 6: 135:195695

REFERENCE 7: 134:366630

REFERENCE 8: 134:178294

REFERENCE 9: 129:175353

REFERENCE 10: 127:242400

L26 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2005 ACS on STN

RN 142623-70-9 REGISTRY

ED Entered STN: 24 Jul 1992

CN Phenol, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)thio]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H9 F17 O S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

REFERENCE 2: 138:320984

REFERENCE 3: 117:101039

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FILE 'HCAPLUS' ENTERED AT 07:12:40 ON 12 APR 2005
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L33 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:60433 HCAPLUS

DN 140:128148

ED Entered STN: 26 Jan 2004

TI A method for preparing new fluorous tagging and scavenging reactants and uses thereof

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Zhang, Wei; Luo, Zhiyong; Nagashima, Tadamichi; Chen, Christine Hiu-Tung;
     Yu, Marvin S.
PΑ
     Fluorous Technologies Incorporated, USA
SO
     PCT Int. Appl., 83 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
IC
     ICM CO7C
     25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
CC
FAN.CNT 1
     PATENT NO.
                        KIND
                               DATE
                                           APPLICATION NO.
     ______
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                               _____
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PΙ
    WO 2004007407
                         A2
                               20040122
                                           WO 2003-US21686
                                                                 20030711 <--
    WO 2004007407
                         A3
                               20041125
        W: CA, JP
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
            IT, LU, MC, NL, PT, RO, SE, SI, SK, TR
     US 2004073054
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                                         US 2003-617431
PRAI US 2002-395067P
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    US 2002-396952P
                         Р
                               20020718
    US 2003-442712P
                         Ρ
                               20030127
    US 2003-442762P
                         Ρ
                               20030127
                         Р
    US 2003-442840P
                               20030127
CLASS
PATENT NO.
                CLASS
                       PATENT FAMILY CLASSIFICATION CODES
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WO 2004007407
                ICM
                       C07C
US 2004073054
                ECLA
                       C07B051/00; C07D213/74; C07D213/74C; C07D217/04;
                       C07D217/06; C07D231/38; C07D265/26B;
                       C07D401/12+211+209C; C07D401/14+239B+231+217;
                       C07D401/14+239B+231+213; C07D403/04+239B+231;
                       C07D403/14+239B+239B+231; C07D417/14+277+239B+231;
                       C07D417/14+285B+239B+231; C07D471/04+239C+221C;
                       C07D487/04+239C+239C+2; C07D491/10+317B+221B;
                       C07B063/02; C07C017/16+22/08; C07C022/08; C07C043/23;
                       C07C045/71+47/575; C07C047/575; C07C053/50; C07C211/14;
                       C07C211/15; C07C213/00; C07C265/04; C07C273/18B2B;
                       C07C311/16; C07C323/20; C07C335/16; C07D207/46;
                       C07D209/14; C07D209/16; C07D211/62
os
    MARPAT 140:128148
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The present invention includes methods and compns. for increasing the fluorous nature of an organic compound, which contains at least one functional group reactive with group X, by reacting it with at least one fluorous compound of formula XCR1R2(C6H5)m[Wp(CH2)nRf]m [wherein X = a leaving group, a nucleophilic group, or an electrophilic group; R1 and R2 = independently H, alkyl, Ph, (C6R5)q(W')q, or (C6H5)m'[Wp'(CH2)n'Rf]m'; m and m' = independently 1-5; n and n' = independently 0-5; p and p' = independently 0 or 1; q = 0-5; W = O, S, NR3, CR4R5, SIR6R7; W' = OR8, SR9, NR1OR11, CR12R13R14, or SiR15R16R17; R3, R4, R5, R8-R14 = independently H, alkyl, aryl, benzyl, or (CH2)n''Rf; R6, R7, R15-R17 = independently alkyl, aryl,

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benzyl, or (CH2)n''Rf; n'' = 0-5; Rf = perfluoroalkyl, a fluorinated either, or a fluorinate amine; with provisos] to produce a fluorous tagged organic compound The increased fluorous nature of the fluorous tagged organic compound may then be used to sep. the fluorous organic compound from untagged reagents, reactants, catalysts, and/or products derived from it. The resultant fluorous tagged organic compound may also be subjected to subsequent chemical transformations, wherein the fluorous nature of the tagged compound is used to increase the ease of separation of the fluorous tagged organic compound from untagged reagents, reactants, catalysts, and/or products derived therefrom, after each chemical transformation. The chemical transformations result in a second fluorous tagged organic compound, which may be reduced by removing the fluorous group thereby producing a second organic compound second organic compound may be employed as a pharmaceutical compound or intermediate or as a combinatorial library component. For example, reaction of 4-(1H,1H,2H,2H-perfluorodecyl)benzyl alc. with phosgene in anhydrous THF, followed by coupling with N-hydroxysuccinimide dicyclohexylamine salt in chloroform and workup, provided I (82%). fluorous tagging scavenging reactant prepn fluoroalkylation; combinatorial library fluoroalkyl benzene deriv prepn Haloalkylation (fluoroalkylation; preparation of new fluorous tagging and scavenging reactants and uses thereof) Scavengers (fluorous electrophilic; preparation of new fluorous tagging and scavenging reactants and uses thereof) Organic compounds, preparation RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (fluorous tagged; preparation of new fluorous tagging and scavenging reactants and uses thereof) Combinatorial library (preparation of new fluorous tagging and scavenging reactants and uses 142010-50-2P 501701-51-5P 514221-87-5P 544418-04-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (fluorous tagging and scavenging compound; preparation of new fluorous tagging and scavenging reactants and uses thereof) 17002-69-6P **494798-73-1P**, 4-[[3-(Perfluorooctyl)propyl]oxy]benza ldehyde 556050-49-8P 649561-59-1P 649561-67-1P 649561-68-2P 649561-73-9P RL: SPN (Synthetic preparation); PREP (Preparation) (fluorous tagging and scavenging compound; preparation of new fluorous tagging and scavenging reactants and uses thereof) 142623-70-9P 501701-48-0P 501701-50-4P 514221-85-3P 514221-86-4P 649561-57-9P 649561-58-0P 649561-66-0P 649561-69-3P 649561-74-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of new fluorous tagging and scavenging reactants and uses thereof) 91-21-4, 1,2,3,4-Tetrahydroisoquinoline 61-54-1, 3-Indoleethanamine 100-07-2, 4-Methoxybenzoyl chloride 103-71-9, Phenyl isocyanate, 103-72-0, Phenyl isothiocyanate 104-84-7, 4-Methylbenzylamine 110-91-8, Morpholine, reactions 111-40-0, Diethylenetriamine 118-48-9, Isatoic anhydride 119-61-9, Benzophenone,

122-01-0, 4-Chlorobenzoyl chloride

637-89-8, 4-Mercaptophenol 701-34-8, 4-Bromobenzenesulfonamide

153-78-6, 2-Aminofluorene

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reactions

2043-53-0 2211-94-1, 2-[(4-Methoxyphenoxy)methyl]oxirane 5424-21-5, 2,4-Dichloro-6-methylpyrimidine 5807-14-7 20154-03-4, 3-Trifluoromethylpyrazole 21652-58-4, 1H,1H,2H-Perfluorodec-1-ene 28777-87-9, Hydroxybenzaldehyde 34143-74-3 34803-66-2, 1-(2-Pyridyl)piperazine 82911-72-6 84358-13-4 89373-67-1 195324-88-0 200112-75-0, 3-(Perfluorooctyl)propyl iodide 356055-77-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of new fluorous tagging and scavenging reactants and uses thereof)

IT 32569-50-9P 32585-51-6P 3083-88-3P 6336-01-2P 35305-46-5P 35305-48-7P 83491-16-1P 89652-23-3P 330865-56-0P 331631-15-3P 333768-48-2P 377767-02-7P 433706-16-2P 501701-52-6P 501701-53-7P 501701-54-8P 501701-55-9P 501701-56-0P 501701-57-1P 501701-58-2P 501701-59-3P 501701-60-6P 501701-61-7P 503429-92-3P 514221-95-5P 514221-96-6P 514221-98-8P 514221-99-9P 514222-01-6P 544418-15-7P 649561-60-4P 649561-61-5P 649561-62-6P 649561-65-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of new fluorous tagging and scavenging reactants and uses thereof)

IT 501701-51-5P 514221-87-5P 544418-04-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorous tagging and scavenging compound; preparation of new fluorous tagging

and scavenging reactants and uses thereof)

RN 501701-51-5 HCAPLUS

CN Pyrimidine, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)sulfonyl]-6-methyl-2-[3-(trifluoromethyl)-1H-pyrazol1-yl]- (9CI) (CA INDEX NAME)

RN 514221-87-5 HCAPLUS

CN 4-Piperidinecarboxylic acid, 1-(4-chlorobenzoyl)-, 4[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]phenyl
ester (9CI) (CA INDEX NAME)

$$F_3C-(CF_2)_7-CH_2-CH_2-S$$

RN 544418-04-4 HCAPLUS

CN 2H-3,1-Benzoxazine-2,4(1H)-dione, 1-(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,1 1-heptadecafluoroundecyl)- (9CI) (CA INDEX NAME)

IT 494798-73-1P, 4-[[3-(Perfluorooctyl)propyl]oxy]benzaldehyde

556050-49-8P 649561-59-1P 649561-67-1P

649561-68-2P 649561-73-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(fluorous tagging and scavenging compound; preparation of new fluorous

tagging

and scavenging reactants and uses thereof)

RN 494798-73-1 HCAPLUS

CN Benzaldehyde, 4-[(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-

heptadecafluoroundecyl)oxy] - (9CI) (CA INDEX NAME)

RN 556050-49-8 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

RN 649561-59-1 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)-9H-fluoren-9-yl]methoxy]carbonyl]oxy]- (9CI) (CA
INDEX NAME)

RN 649561-67-1 HCAPLUS

CN Benzene, 1-(chlorodiphenylmethyl)-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{(CF}_2)} & 7\text{--}\text{CF}_3 \\ \text{Ph} & \text{--}\text{Cl} & \text{--}\text{Ph} \end{array}$$

RN 649561-68-2 HCAPLUS

CN 2H-Pyrimido[1,2-a]pyrimidine, 1-(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecyl)-1,3,4,6,7,8-hexahydro-(9CI) (CA INDEX NAME)

RN 649561-73-9 HCAPLUS

CN Benzenesulfonamide, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{(CF}_2)}_{7}\text{-}\text{CF}_3\\ \\ \text{H}_2\text{N-}\underset{\text{O}}{\text{S}} & \\ \\ \end{array}$$

IT 142623-70-9P 501701-48-0P 501701-50-4P
514221-85-3P 514221-86-4P 649561-57-9P
649561-58-0P 649561-66-0P 649561-74-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of new fluorous tagging and scavenging reactants and uses thereof)

RN 142623-70-9 HCAPLUS

CN Phenol, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]- (9CI) (CA INDEX NAME)

RN 501701-48-0 HCAPLUS

CN Pyrimidine, 2-chloro-4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]-6-methyl- (9CI) (CA INDEX NAME)

RN 501701-50-4 HCAPLUS

CN Pyrimidine, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]-6-methyl-2-[3-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

RN 514221-85-3 HCAPLUS

CN 1,4-Piperidinedicarboxylic acid, 1-(1,1-dimethylethyl)
4-[4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]phen
yl] ester (9CI) (CA INDEX NAME)

$$t-BuO-C$$
 $S-CH_2-CH_2-(CF_2)_7-CF_3$

RN 514221-86-4 HCAPLUS

CN 4-Piperidinecarboxylic acid, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)thio]phenyl ester (9CI) (CA INDEX NAME)

RN 649561-57-9 HCAPLUS

CN 9H-Fluorene, 2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decenyl)- (9CI) (CA INDEX NAME)

RN 649561-58-0 HCAPLUS

CN 9H-Fluorene-9-methanol, 2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

RN 649561-66-0 HCAPLUS

CN Benzenemethanol, $4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-<math>\alpha, \alpha-diphenyl-$ (9CI) (CA INDEX NAME)

RN 649561-74-0 HCAPLUS

CN Benzenesulfonamide, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decenyl)- (9CI) (CA INDEX NAME)

IT 195324-88-0 356055-77-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of new fluorous tagging and scavenging reactants and uses
 thereof)

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RN 195324-88-0 HCAPLUS
CN Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) - (9CI) (CA INDEX NAME)

CH2-CH2-(CF2)7-CF3

RN 356055-77-1 HCAPLUS
CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) - (9CI) (CA INDEX NAME)

CH2-CH2-(CF2)7-CF3
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ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN .
L33
     2003:154376 HCAPLUS
AN
DN
     138:204515
ED
     Entered STN: 28 Feb 2003
     Fluorous nucleophilic substitution of alcohols and reagents for use
TΤ
     therein, specifically, perfluoroalkyl-containing phosphines and
     azodicarboxylates as polyfluorinated reagents for the Mitsunobu reaction
IN
     Curran, Dennis P.; Dandapani, Sivaraman
PA
     University of Pittsburgh, USA
SO
     PCT Int. Appl., 51 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
IC
     ICM C07B063-00
     ICS C07B045-00; C07B041-12; C07C067-08; C07C303-40; C07C311-58
     21-2 (General Organic Chemistry)
     Section cross-reference(s): 45
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                                            WO 2002-US26045
PΙ
     WO 2003016246
                          A1.
                                20030227
                                                                    20020815 <--
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
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     US 6806357
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
                                                                    20020815 <--
     JP 2005508890
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                                           JP 2003-521175
PRAI US 2001-932903
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20020815

WO 2002-US26045

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CLASS
PATENT NO.
                CLASS PATENT FAMILY CLASSIFICATION CODES
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WO 2003016246
                ICM
                      C07B063-00
                      C07B045-00; C07B041-12; C07C067-08; C07C303-40;
                ICS
                      C07C311-58
                      C07B041/12; C07B063/00; C07C067/08; C07C281/02;
WO 2003016246
                ECLA
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                      C07C281/20; C07C303/40
                      C07B041/12; C07B063/00; C07C067/08; C07C281/02;
US 6806357
                ECLA
                      C07C281/20; C07C303/40
                                                                        <--
JP 2005508890
                FTERM
                      4C204/AB20; 4C204/BB10; 4C204/CB04; 4C204/DB01;
                      4C204/EB01; 4C204/FB03; 4C204/FB04; 4C204/FB10;
                      4C204/GB01; 4H006/AA02; 4H006/AC48; 4H006/AC90;
                      4H006/KA06
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OS CASREACT 138:204515; MARPAT 138:204515

AB Phosphine and azodicarboxylate reagents containing perfluoroalkyl groups are employed in the Mitsunobu reaction of alcs. with acids, imides, and sulfonamides. Claims cover a method of effecting a nucleophilic substitution of an alc. to produce a target product which involves reaction of the alc. with a nucleophile, using an azodicarboxylate and a phosphine which contain between them at least one "fluorous tag", i.e., a perfluoroalkyl group. These fluorinated reagents and the byproducts they form are readily removed from the reaction mixture by separation techniques which

target perfluorinated substances, e.g., liquid-liquid or solid-liquid extraction

Such "fluorous" separation techniques are superior to standard chromatog. separation

methods, which are less effective and are undesirable for both industrial and combinatorial use. Several examples of both types of Mitsunobu reagents were prepared and used. For instance, CF3(CF2)5CH2CH2I (RFI) reacted with Zn in THF, and then with 4-IC6H4Br in the presence of Pd(PPh3)4, to give 53% 4-RFC6H4Br. This bromide was lithiated with tert-BuLi and then coupled with PhPC12 to give 81% yield of the triarylphosphine (4-RFC6H4)2PPh (I). Similarly, the alc. CF3(CF2)5CH2CH2OH (RFOH) was esterified with carbonyldiimidazole and coupled with hydrazine hydrochloride in the presence of Et3N to give 85% RFO2CNHNHCO2RF. Oxidation of this hydrazine derivative with Br2 in the

of pyridine gave 100% RFO2CN:NCO2RF (II). Mitsunobu reaction of EtOH with 3,5-dinitrobenzoic acid was carried out in THF using I and II, stirring overnight at room temperature Separation of the reaction mixture using fluorous

reverse-phase silica gel chromatog., eluting with 80% MeOH, gave (1) an organic fraction containing Et 3,5-dinitrobenzoate in 92% yield and 100% purity,

and (2) a mixture of fluorous byproducts consisting of the corresponding hydrazine (80%) and phosphine oxide (86%). The byproducts are easily recycled by oxidation and reduction, resp., in nearly quant. yields. A variety of other reactants, reagents, exptl. conditions, and procedural variants were studied.

ST fluorous nucleophilic substitution alc; Mitsunobu perfluoroalkyl phosphine azodicarboxylate reagent; phthalimide nitrobenzoate toluenesulfonamide nitrophenylbutyrate Mitsunobu alc fluorous reagent; combinatorial industrial chem Mitsunobu reagent

IT Dehydration reaction

(Mitsunobu reaction; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents)

IT Alkylation

Esterification

Substitution reaction, nucleophilic

(Mitsunobu; nucleophilic substitution of alcs. by Mitsunobu reaction

using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) TΤ Dehydration reaction (agents; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) IT (perfluoroalkyl; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) Esters, preparation IT RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (products; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) IT Imides Sulfonamides RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (reactants and products; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) Alcohols, reactions Carboxylic acids, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (reactants; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) TT Combinatorial chemistry (reagents for; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) TΤ 304-17-6P, N-Isopropylphthalimide 318-49-0P, N-(p-550-44-7P, N-Methylphthalimide Fluorobenzyl)phthalimide 618-71-3P. Ethyl 3,5-dinitrobenzoate 2702-58-1P, Methyl 3,5-dinitrobenzoate 5022-29-7P, N-Ethylphthalimide 5428-09-1P, N-Allylphthalimide 10477-99-3P, Isopropyl 3,5-dinitrobenzoate 20637-02-9P, Methyl 4-(4-nitrophenyl)butyrate 54619-90-8P, Allyl 3,5-dinitrobenzoate 56805-36-8P, N-Methyl-N-(tert-butoxycarbonyl)-p-toluenesulfonamide 462996-05-0P, p-Fluorobenzyl 3,5-dinitrobenzoate 462996-06-1P, N-Allyl-N-(tert-butoxycarbonyl)-p-toluenesulfonamide 462996-07-2P, N-(p-Fluorobenzyl)-N-(tert-butoxycarbonyl)-p-toluenesulfonamide 462996-08-3P, Allyl 4-(4-nitrophenyl)butyrate 462996-09-4P, p-Fluorobenzyl 4-(4-nitrophenyl) butyrate RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (Mitsunobu product; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) 64-17-5, Ethanol, reactions 67-56-1, Methanol, reactions 67-63-0, 85-41-6, Phthalimide Isopropanol, reactions 99-34-3, 3,5-Dinitrobenzoic acid 107-18-6, Allyl alcohol, reactions 459-56-3, 5600-62-4, 4-(4-Nitrophenyl) butyric acid p-Fluorobenzyl alcohol 18303-04-3, N-(tert-Butoxycarbonyl)-p-toluenesulfonamide RL: RCT (Reactant); RACT (Reactant or reagent) (Mitsunobu reactant; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) IT 290827-85-9P, Phenylbis[4-(3,3,4,4,5,5,6,6,7,7,8,8,8tridecafluorooctyl)phenyl]phosphane oxide RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (byproduct; nucleophilic substitution of alcs. by Mitsunobu reaction using perfluoroalkyl-containing phosphine and azodicarboxylate reagents) IT 290827-94-0P, Phenylbis[4-(3,3,4,4,5,5,6,6,7,7,8,8,8tridecafluorooctyl)phenyl]phosphane 452912-11-7P, Bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) azodicarboxylate

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462996-01-6P, Bis(4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl
                       462996-04-9P, Diphenyl [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,1
     azodicarboxylate
     0,10,10-heptadecafluorodecyl)phenyl]phosphane
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
        (invention Mitsunobu reagent; nucleophilic substitution of alcs. by
       Mitsunobu reaction using perfluoroalkyl-containing phosphine and
        azodicarboxylate reagents)
     1972-28-7, DEAD
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (non-invention Mitsunobu reagent; nucleophilic substitution of alcs. by
       Mitsunobu reaction using perfluoroalkyl-containing phosphine and
       azodicarboxylate reagents)
     936-58-3P, \alpha-Allylbenzyl alcohol 120848-76-2P,
     2-(Piperidin-4-ylcarbonyl)-1,2,3,4-tetrahydroisoquinoline
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (other product; nucleophilic substitution of alcs. by Mitsunobu
        reaction using perfluoroalkyl-containing phosphine and azodicarboxylate
       reagents)
     100-52-7, Benzaldehyde, reactions
                                       192212-66-1,
    Allyltris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)stannane
     217805-02-2, Allyltris(4,4,5,5,6,6,7,7,8,8,9,9,9-
     tridecafluorononyl) stannane 350716-46-0, 1,1-
     Bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)ethyl
     4-[(1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidine-1-carboxylate
     350716-52-8, 1,1-Bis(4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl)ethyl
     4-[(1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidine-1-carboxylate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (other reactant; nucleophilic substitution of alcs. by Mitsunobu
        reaction using perfluoroalkyl-containing phosphine and azodicarboxylate
        reagents)
     452912-12-8P, Bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)
     hydrazine-1,2-dicarboxylate
     RL: BYP (Byproduct); IMF (Industrial manufacture); RCT (Reactant); SPN
     (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
        (reagent intermediate and byproduct; nucleophilic substitution of alcs.
       by Mitsunobu reaction using perfluoroalkyl-containing phosphine and
        azodicarboxylate reagents)
     80806-68-4P, 4,4,5,5,6,6,7,7,8,8,9,9,9-Tridecafluorononan-1-ol
     195324-87-9P, 1-Bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,8-
     tridecafluorooctyl)benzene 195324-88-0P, 1-Bromo-4-
     (3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)benzene
     462995-97-7P, Bis(4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl
     hydrazine-1,2-dicarboxylate
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
        (reagent intermediate; nucleophilic substitution of alcs. by Mitsunobu
        reaction using perfluoroalkyl-containing phosphine and azodicarboxylate
        reagents)
     530-62-1, 1,1'-Carbonyldiimidazole
                                          589-87-7, 1-Bromo-4-iodobenzene
     644-97-3, Dichlorophenylphosphine 647-42-7, 3,3,4,4,5,5,6,6,7,7,8,8,8-
                              1079-66-9 2043-53-0,
     Tridecafluoro-1-octanol
     1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-Heptadecafluoro-10-iododecane
     2043-57-4, 1,1,1,2,2,3,3,4,4,5,5,6,6,-Tridecafluoro-8-iodooctane
     2644-70-4, Hydrazine monohydrochloride
                                             38550-44-6, 2-Iodo-
     4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononan-1-ol
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reagent precursor; nucleophilic substitution of alcs. by Mitsunobu
        reaction using perfluoroalkyl-containing phosphine and azodicarboxylate
        reagents)
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     195324-88-0P, 1-Bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
     heptadecafluorodecyl) benzene
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
        (reagent intermediate; nucleophilic substitution of alcs. by Mitsunobu
        reaction using perfluoroalkyl-containing phosphine and azodicarboxylate
        reagents)
RN
     195324-88-0 HCAPLUS
CN
     Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
     heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
           CH_2 - CH_2 - (CF_2)_7 - CF_3
     ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
     2002:640921 HCAPLUS
     138:136691
DN
     Entered STN: 26 Aug 2002
ED
     Fluorous-tethered amine bases for organic and parallel synthesis: scope
ΤI
     and limitations
ΑU
     Lindsley, Craig W.; Zhao, Zhijian; Leister, William H.; Strauss, Kimberly
     Technology Enabled Synthesis Group, Department of Medicinal Chemistry,
CS
     Merck Research Laboratories, West Point, PA, 19486, USA
SO
     Tetrahedron Letters (2002), 43(36), 6319-6323
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The synthesis of fluorous-tethered amine bases is described. These novel

(fluoro-containing; preparation of pure fluorous-tethered amine reagents for

fluorous-tethered reagents promote reactions, remove acidic byproducts, and scavenge electrophiles. They are readily separated from the reaction mixture by solid phase extraction on a novel mixed sorbent SPE (SCX/fluorous

reaction promoters, acidic byproduct removal, and as electrophile

(preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers)

(preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers)

(scavengers for; preparation of pure fluorous-tethered amine reagents for

silica gel) delivering products in high yields and purities.

RL: PUR (Purification or recovery); RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RL: PUR (Purification or recovery); RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

CODEN: TELEAY; ISSN: 0040-4039

21-2 (General Organic Chemistry)

fluorous tethered amine reagent prepn

Elsevier Science Ltd.

CASREACT 138:136691

Amines, preparation

scavengers)

Scavengers

Electrophiles

Reagents

Acylation catalysts

Journal English

PB DT

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647-42-7

reaction promoters, acidic byproduct removal, and as electrophile scavengers) 3647-71-0 RL: RCT (Reactant); RACT (Reactant or reagent) (acylation and sulfonylation of; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 51-45-6, 1H-Imidazole-4-ethanamine, reactions 104-78-9 123-00-2, 4-Morpholinepropanamine 4963-47-7 13258-63-4, 4-Pyridineethanamine RL: RCT (Reactant); RACT (Reactant or reagent) (acylation of; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 335-64-8 RL: RCT (Reactant); RACT (Reactant or reagent) (acylation with; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 307-29-9 RL: MSC (Miscellaneous) (preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 494798-79-7P 494798-80-0P 494798-74-2P 494798-78-6P 494798-81-1P 494798-82-2P 494798-83-3P RL: PUR (Purification or recovery); RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 3278-14-6P 87736-74-1P 470475-47-9P RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation) (preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 98-88-4, Benzoyl chloride 1648-99-3 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 873-75-6, p-Bromobenzyl alcohol RL: RCT (Reactant); RACT (Reactant or reagent) (protection of; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 64-04-0, Benzeneethanamine RL: RCT (Reactant); RACT (Reactant or reagent) (reaction with benzoyl chloride; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 110-91-8, Morpholine, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (reductive amination of aldehyde with; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers) 494798-73-1 RL: RCT (Reactant); RACT (Reactant or reagent) (reductive amination of; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers)

RL: RCT (Reactant); RACT (Reactant or reagent) (scavenger; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers)

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- (12) Zhang, W; Tetrahedron 2002, V58, P3871 HCAPLUS
- IT 494798-73-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reductive amination of; preparation of pure fluorous-tethered amine reagents for reaction promoters, acidic byproduct removal, and as electrophile scavengers)

- RN 494798-73-1 HCAPLUS
- CN Benzaldehyde, 4-[(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11heptadecafluoroundecyl)oxy]- (9CI) (CA INDEX NAME)

- L33 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:337996 HCAPLUS
- DN 137:262818
- ED Entered STN: 07 May 2002
- TI Fluorous Mitsunobu reagents and reactions
- AU Dandapani, Sivaraman; Curran, Dennis P.
- CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
- SO Tetrahedron (2002), 58(20), 3855-3864 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier Science Ltd.
- DT Journal
- LA English

of

- CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds) Section cross-reference(s): 23
- OS CASREACT 137:262818
- A fully fluorous Mitsunobu reaction procedure is introduced using fluorous triphenylphosphines [4-(C6F13CH2CH2)C6H4]2PPh (I) and 4-(C8F17CH2CH2)C6H4PPh2 (II) and a fluorous azodicarboxylate C6F13CH2CH2OC(:0)N:NCOOCH2CH2C6F13 (III). The modified Mitsunobu procedure is used for the preparation of amines, imides, and esters by Mitsunobu reactions of 3,5-dinitro- and 4-nitrobenzoic acids, 4-(4-nitrophenyl)butanoic acid, phthalimide, and N-(tert-butoxycarbonyl)-4-toluenesulfonamide with methanol, ethanol, allyl alc., and 4-fluorobenzyl alc. Et anti-2-methyl-3-hydroxybutanoate and cholestanol are also esterified with clean inversion using II and III as Mitsunobu reagents. The order of addition of the reagents affects the reaction yields significantly; addition of III to a solution of I in THF followed by addition

the alc. and addition of the desired nucleophile gave the highest yields for Mitsunobu reactions. The fluorous hydrazinecarboxylate and fluorous

triphenylphosphine oxide byproducts are removed from the reaction mixture by chromatog. on fluorous silica gel; III and I are then regenerated from the separated byproducts by oxidation with bromine and reduction with the complex

οf

dimethylamine and alane, resp. This procedure allows the ready separation of the difficultly separated triphenylphosphine oxide and hydrazinecarboxylate byproducts from Mitsunobu reactions.

ST fluorous triphenylphosphine prepn reagent Mitsunobu reaction; fluorinated azodicarboxylate prepn reagent Mitsunobu reaction; amide prepn; ester prepn; Mitsunobu reaction alc arom acid phthalimide sulfonamide fluorous reagent; removal byproduct regeneration fluorous triphenylphosphine azodicarboxylate Mitsunobu reaction

IT Substitution reaction, nucleophilic

(Mitsunobu; preparation of fluorous triphenylphosphines and fluorous azodicarboxylates as readily separated and regenerated reagents for Mitsunobu reaction of alcs.)

IT Alcohols, reactions

Carboxylic acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fluorous triphenylphosphines and fluorous azodicarboxylates as readily separated and regenerated reagents for Mitsunobu reaction of alcs.)

IT Esters, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of fluorous triphenylphosphines and fluorous azodicarboxylates as readily separated and regenerated reagents for Mitsunobu reaction of alcs.)

IT 375-01-9 80806-68-4 83310-97-8 148043-73-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fluorous azodicarboxylates as readily separated and regenerated

reagents for Mitsunobu nucleophilic substitution reactions of alcs.)

IT 452912-12-8P 462995-97-7P 462995-98-8P 462995-99-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fluorous azodicarboxylates as readily separated and regenerated $% \left(1\right) =\left(1\right) +\left(1\right) +\left($

reagents for Mitsunobu nucleophilic substitution reactions of alcs.) IT 452912-11-7P

RL: RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

reagents for Mitsunobu nucleophilic substitution reactions of alcs.)
T 462996-00-5P 462996-01-6P 462996-02-7P 462996-03-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of fluorous azodicarboxylates as readily separated and regenerated

reagents for Mitsunobu nucleophilic substitution reactions of alcs.)

IT 80-97-7, Cholestanol 85-41-6, Phthalimide 99-34-3, 3,5-Dinitrobenzoic acid 459-56-3, 4-Fluorobenzyl alcohol 647-42-7 5600-62-4,

4-(4-Nitrophenyl) butanoic acid 18303-04-3 51898-36-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of fluorous triphenylphosphines and fluorous azodicarboxylates as readily separated and regenerated reagents for Mitsunobu nucleophilic substitution reactions of alcs.)

IT 290827-94-0

RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of fluorous triphenylphosphines and fluorous azodicarboxylates as readily separated and regenerated reagents for Mitsunobu nucleophilic substitution reactions of alcs.)

IT 304-17-6P, N-Isopropylphthalimide 318-49-0P, N-(p-Fluorobenzyl)phthalimide 550-44-7P, N-Methylphthalimide 618-71-3P, IT

IT

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Ethyl 3,5-dinitrobenzoate
                                 2702-58-1P, Methyl 3,5-dinitrobenzoate
     5022-29-7P, N-Ethylphthalimide
                                    5428-09-1P, N-Allylphthalimide
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                                                 20637-02-9P
                                 56805-36-8P 96946-70-2P
     Allyl 3,5-dinitrobenzoate
                                                             462996-05-0P
                    462996-07-2P
                                   462996-08-3P
                                                 462996-09-4P
     462996-06-1P
                                                                 462996-10-7P
     462996-11-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of fluorous triphenylphosphines and fluorous azodicarboxylates
        as readily separated and reqenerated reagents for Mitsunobu nucleophilic
        substitution reactions of alcs.)
     1079-66-9, Chlorodiphenylphosphine 195324-88-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of fluorous triphenylphosphines as readily separated and
        regenerated reagents for Mitsunobu nucleophilic substitution reactions
        of alcs.)
     462996-04-9P
     RL: RGT (Reagent); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of fluorous triphenylphosphines as readily separated and
        regenerated reagents for Mitsunobu nucleophilic substitution reactions
        of alcs.)
     290827-85-9P
     RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or
     reagent)
        (regeneration of a fluorous azodicarboxylate from a
       hydrazinecarboxylate byproduct of Mitsunobu nucleophilic substitution
       reactions of alcs. with a fluorous azodicarboxylate reagent)
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IT
     195324-88-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of fluorous triphenylphosphines as readily separated and
        regenerated reagents for Mitsunobu nucleophilic substitution reactions
        of alcs.)
     195324-88-0 HCAPLUS
RN
    Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
CN
    heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
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    ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
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     135:195695
DN
     Entered STN: 24 Aug 2001
ED
     Fluorous reaction and separation methods
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IN
     Curran, Dennis P.; De Frutos Garcia, Oscar; Oderaotoshi, Yoji
PΑ
     University of Pittsburgh, USA
SO
     PCT Int. Appl., 77 pp.
     CODEN: PIXXD2
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IC
     ICM G01N027-26
     31-5 (Alkaloids)
     Section cross-reference(s): 21, 29
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            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    US 6749756
                         B1
                               20040615
                                         US 2000-506779
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    CA 2400439
                         AΑ
                               20010823
                                           CA 2001-2400439
                         A1
    EP 1269170
                               20030102
                                           EP 2001-910849
                                                                  20010216 <--
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR JP 2001-560670 JP 2003523350 T2 20030805 20010216 <--US 2004-831087 US 2004197829 **A1** 20041007 20040423 <--PRAI US 2000-506779 Α 20000218 <--WO 2001-US5065 W 20010216 CLASS PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES ----WO 2001061332 ICM G01N027-26 ECLA G01N027/447B3A2 US 6749756 US 2004197829 ECLA G01N027/447B3A2 <--

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$$\mathbb{R}^1$$
 \mathbb{N} \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^3 \mathbb{R}^4 \mathbb{R}^4

AB The present invention provides a fluorous-tagging strategy comprising the steps of: a. tagging a first organic compound with a first tagging moiety to result in a first tagged compound; b. tagging at least a second organic compound

with a second tagging moiety different from the first tagging moiety to result in a second tagged compound; and c. separating the first tagged compound from a mixture including the second tagged compound using a separation technique

based upon differences between the first tagging moiety and the second tagging moiety, in the synthesis and separation of mixts. of organic compds. including analogs of mappicine, such as, [I; R1 = H, aryl, SiMe2Bu-t; R2 = alkyl, CH2Ph; R3 = alkyl; R4 = alkyl, fluoroalkyl]. Thus, mappicine analogs, such as, I [R1 = H, Ph, SiMe2Bu-t; R2 = Et, Bu-t, CH2Ph; R3 = Me, (Me)2CH,; R4 = C6H13, C4F9, C6F13, C8F17, C10F21] were prepared via radical cyclization of N-alkylated pyridone [II; R1 = H, Ph, SiMe2Bu-t; R2 = Et, Bu-t, CH2Ph; R3 = Me, (Me)2CH,; R4 = C6H13, C4F9, C6F13, C8F17, C10F21] (also prepared) and 4-methylphenyl isonitrile and separated by preparative HPLC with a FluofixTM column.

ST fluorous tagging strategy org compd prepn mappicine sepn analog; cyclization radical prepn mappicine analog pyridone methylphenyl isonitrile

IT Combinatorial library

(fluorous mixture synthesis, a fluorous-tagging strategy for synthesis and separation of mixts. of organic compds.)

IT Alkaloids, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(fluorous-tagging strategy for synthesis and separation of mixts. of mappicine analog)

IT Organic compounds, preparation

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(fluorous-tagging strategy for synthesis and separation of mixts. of organic compds.)

IT Silanes

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

```
(Reactant or reagent)
        (haloalkyl; fluorous-tagging strategy for synthesis and separation of mixts.
        of organic compds.)
TT
     Preparative liquid chromatography
        (high-performance; with Fluofix column for separation of mixts. of organic
        compds.)
IT
     Electrophoresis
     Ion exclusion chromatography
        (in separation of fluorous tagged products)
IT
     Reversed phase chromatography
        (in separation of mixts. of organic compds.)
IT
        (preparative; with Fluofix column for separation of mixts. of organic
compds.)
IT
     Combinatorial chemistry
        (use of fluorous-tagging strategy for synthesis and separation of mixts. of
        organic compds. in relation to)
IT
     195324-87-9P 195324-88-0P
                                 305816-08-4P
                                                356055-74-8P
                                                356055-79-3P
     356055-76-0P 356055-77-1P
                                 356055-78-2P
                                   356055-86-2P
                                                  356055-87-3P
                                                                  356056-17-2P
     356055-83-9P
                    356055-85-1P
     356056-18-3P
                    356056-19-4P
                                   356056-20-7P
                                                  356056-21-8P
                                                                  356056-44-5P
     356056-45-6P
     RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
        (fluorous-tagging strategy for synthesis and separation of mixts. of organic
        compds.)
                                        305816-04-0P
                                                        356055-80-6P
IT
     54318-59-1DP, Mappicine, analogs
     356055-81-7P
                    356055-82-8P
                                   356055-84-0P
                                                  356055-88-4P
                                                                  356055-89-5P
     356055-90-8P
                    356055-91-9P
                                   356055-92-0P
                                                   356055-93-1P
                                                                  356055-94-2P
                    356055-96-4P
     356055-95-3P
                                   356055-97-5P
                                                  356055-98-6P
                                                                  356055-99-7P
                    356056-01-4P
                                   356056-02-5P
                                                  356056-03-6P
                                                                  356056-04-7P
     356056-00-3P
                    356056-06-9P
                                   356056-07-0P
                                                  356056-08-1P
                                                                  356056-09-2P
     356056-05-8P
                    356056-23-0P
                                   356056-24-1P
                                                  356056-25-2P
                                                                  356056-26-3P
     356056-22-9P
                    356056-28-5P
                                   356056-29-6P
                                                  356056-30-9P
                                                                  356056-31-0P
     356056-27-4P
     356056-32-1P
                    356056-33-2P
                                   356056-34-3P
                                                  356056-35-4P
                                                                  356056-36-5P
                    356056-38-7P
                                   356056-39-8P
                                                  356056-40-1P
                                                                  356056-41-2P
     356056-37-6P
     RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP
     (Preparation)
        (fluorous-tagging strategy for synthesis and separation of mixts. of organic
        compds.)
IT
     91-60-1, 2-Naphthalenethiol
                                   97-63-2, Ethyl methacrylate
                                                                  106-93-4,
                        106-96-7, Propargyl bromide
                                                       108-98-5, Benzenethiol,
     1,2-Dibromoethane
                                                    623-70-1, trans-Ethyl
     reactions
                 589-87-7, 1-Bromo-4-iodobenzene
                                                    1493-13-6,
                 696-63-9, 4-Methoxybenzenethiol
     crotonate
     Trifluoromethanesulfonic acid
                                    1794-48-5
                                                 2043-53-0
                                                             2043-54-1
                             2227-29-4, Chlorodiisopropylsilane
     2043-55-2
                 2043-57-4
                                                                   2396-68-1,
                                7175-47-5, 4-Methylphenyl isonitrile
     4-tert-Butylbenzenethiol
     7790-99-0, Iodine chloride (ICl)
                                        18162-84-0, Dimethyl octylsilyl
                27829-72-7, trans-Ethyl 2-hexenoate
                                                       131365-11-2
                                                                    174092-75-2
     chloride
     340128-72-5
                   356056-42-3
                                 356056-43-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (fluorous-tagging strategy for synthesis and separation of mixts. of organic
        compds.)
IT
     305816-05-1P
                    305816-06-2P
                                   305816-07-3P
                                                   305816-15-3P
                                                                  305816-17-5P
                    305816-21-1P
                                   305816-25-5P
                                                   305816-37-9P
                                                                  356056-10-5P
     305816-19-7P
     356056-11-6P
                    356056-12-7P
                                   356056-13-8P
                                                   356056-14-9P
                                                                  356056-15-0P
     356056-16-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (fluorous-tagging strategy for synthesis and separation of mixts. of organic
        compds.)
              THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
RE
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- (1) Jackson; US 5340453 A 1994 HCAPLUS
- (2) Wang; US 4454233 A 1984 HCAPLUS
- IT 195324-88-0P 356055-77-1P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorous-tagging strategy for synthesis and separation of mixts. of organic compds.)

RN 195324-88-0 HCAPLUS

CN Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

RN 356055-77-1 HCAPLUS

CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

$$CH_2-CH_2-(CF_2)_7-CF_3$$

$$HO-CH_2$$

- L33 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 2001:419502 HCAPLUS
- DN 135:256798
- ED Entered STN: 11 Jun 2001
- TI Thiol additions to acrylates by fluorous mixture synthesis: relative control of elution order in demixing by the fluorous tag and the thiol substituent
- AU Curran, D. P.; Oderaotoshi, Y.
- CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260,
- SO Tetrahedron (2001), 57(24), 5243-5253 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- CC 21-2 (General Organic Chemistry)
- OS CASREACT 135:256798
- All possible combinations of a series of three fluorous benzyl tags and three acrylates have been made. The resulting acrylate esters were combined in groups of three (one of each tag) and the resulting mixts. were reacted with a mixture of four thiols under standard conditions to effect conjugate addition Anal. of the resulting libraries by fluorous HPLC showed a primary separation based on the tag and revealed reliable secondary sepns. based on the thiol and the acrylate. The primary and secondary sepns. were used together in a preparative 'mixture of mixts.' experiment in which one of the tagged acrylate mixts. was reacted with a mixture of three thiols. The resulting nine component mixture was demixed by fluorous and reverse phase HPLC and then detagged to give all nine final products in pure form. Information on the effectiveness of fluorous tags in fluorous mixture synthesis was gained by reacting mixts. of tagged acrylates with mixts. of thiols followed by demixing.

```
ST
     thiol addn acrylate fluorous mixt
IT
     Addition reaction
        (thiol addns. to acrylates by fluorous mixture synthesis)
     Thiols (organic), reactions
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (thiol addns. to acrylates by fluorous mixture synthesis)
             91-60-1, 2-Naphthalenethiol
IT
                                             108-98-5, Thiophenol, reactions
     80-62-6
     589-87-7, 1-Bromo-4-iodobenzene 623-70-1
                                                 696-63-9,
                             2396-68-1, 4-tert-Butylbenzenethiol
                                                                    13894-63-8
     4-Methoxybenzenethiol
     356055-76-0 356055-77-1
                               356055-78-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (thiol addns. to acrylates by fluorous mixture synthesis)
TT
     195324-87-9P 195324-88-0P
                                 356055-74-8P
                                                 356055-79-3P
     356055-80-6P
                    356055-81-7P
                                   356055-82-8P
                                                   356055-83-9P
                                                                  356055-84-0P
     356055-85-1P
                    356055-86-2P
                                   356055-87-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (thiol addns. to acrylates by fluorous mixture synthesis)
IT
     356055-88-4P
                    356055-89-5P
                                   356055-90-8P
                                                   356055-91-9P
                                                                  356055-92-0P
     356055-93-1P
                    356055-94-2P
                                   356055-95-3P
                                                   356055-96-4P
                                                                  356055-97-5P
     356055-98-6P
                    356055-99-7P
                                   356056-00-3P
                                                   356056-01-4P
                                                                  356056-02-5P
     356056-03-6P
                    356056-04-7P
                                   356056-05-8P
                                                   356056-06-9P
                                                                  356056-07-0P
     356056-08-1P
                    356056-09-2P
                                   356056-27-4P
                                                   356056-28-5P
                                                                  356056-29-6P
     356056-30-9P
                    356056-31-0P
                                   356056-32-1P
                                                   356056-33-2P
                                                                  356056-34-3P
     356056-35-4P
                    356056-36-5P
                                   356056-37-6P
                                                   356056-38-7P
                                                                  356056-39-8P
     356056-40-1P
                    361448-65-9P
                                   529484-63-7P
                                                   529484-65-9P
                                                                  529484-70-6P
     529484-71-7P
                    529484-72-8P
                                   529484-73-9P
                                                   529484-74-0P
                                                                  529484-79-5P
     529484-80-8P
                    529484-81-9P
                                   529484-82-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (thiol addns. to acrylates by fluorous mixture synthesis)
RE.CNT
              THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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(13) Ryu, I; Tetrahedron 2001, V42, P947 HCAPLUS
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(15) Zhang, Q; J Org Chem 2000, V65, P8866 HCAPLUS
IT
     356055-77-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (thiol addns. to acrylates by fluorous mixture synthesis)
RN
     356055-77-1 HCAPLUS
CN
     Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
     heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
```

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

```
(Reactant or reagent)
        (thiol addns. to acrylates by fluorous mixture synthesis)
RN
     195324-88-0 HCAPLUS
     Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
CN
     heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
           CH_2 - CH_2 - (CF_2)_7 - CF_3
Br
     ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
     2001:400120 HCAPLUS
     135:166911
     Entered STN: 05 Jun 2001
ED
     Synthesis, Reactivity, and Metal Complexes of Fluorous Triarylphosphines
TI
     of the Formula P(p-C6H4(CH2)3(CF2)n-1CF3)3 (n = 6, 8, 10)
ΑU
     Soos, Tibor; Bennett, Byron L.; Rutherford, Drew; Barthel-Rosa, Luis P.;
     Gladysz, J. A.
CS
     Institut fuer Organische Chemie, Friedrich-Alexander Universitaet
     Erlangen-Nuernberg, Erlangen, 91054, Germany
SO
     Organometallics (2001), 20(14), 3079-3086
     CODEN: ORGND7; ISSN: 0276-7333
PB
     American Chemical Society
DT
     Journal
     English
T.A
CC
     29-13 (Organometallic and Organometalloidal Compounds)
     Section cross-reference(s): 24, 67
os
     CASREACT 135:166911
AB
     Reactions of p-BrC6H4CH:O with Wittig reagents derived from
     [Ph3PCH2CH2Rfn]+I-(Rfn = (CF2)n-1CF3; n = 6 (6a), 8 (6b), 10 (6c)) give
     p-BrC6H4CH:CHCH2Rfn (86-93%), which are treated with H2 and Wilkinson's
     catalyst to yield p-BrC6H4(CH2)3Rfn (91-94%). Reactions with n-BuLi and
     PC13 (0.33 equiv) give, after workup, mixts. of the title compds. (9a-c)
     and the corresponding phosphine oxides (10a-c). Treatment with H2O2 gives
     pure 10 (a/b/c 88/57/24%), which are reduced with Cl3SiH/Et3N to 9 (a/b/c
     69/82/43%). Fluorous phase affinities increase with perfluoroalkyl chain
     length, as quantified by CF3C6F11/toluene partition coeffs. (9a,
     19.5:80.5; 9b, 66.6:33.4). Reaction of 9b, [Ir(COD)(μ-Cl)]2, and CO
     gives trans-Ir(CO)(Cl)[P(p-C6H4(CH2)3Rf8)3]2 (76%). The IR \nuCO value
     is only slightly greater than that of Vaska's complex (1958 vs 1952 cm-1),
     indicating nearly negligible inductive effects of the perfluoroalkyl
     groups. Reaction of 9b and [Rh(COD)(\mu-C1)]2 yields
     Rh[P(p-C6H4(CH2)3Rf8)3]3(Cl) (82-93%), which gives small equilibrium amts. of
     [Rh[P(p-C6H4(CH2)3Rf8)3]2(\mu-Cl)]2 and 9b in solution, and catalyzes the
     hydrogenation of alkenes under both biphasic (CF3C6F11/toluene) and
     monophasic (CF3C6H5) conditions.
     fluorous triaryl phosphine prepn reaction rhodium iridium cyclooctadiene
ST
     chloride; hydrogenation catalyst fluorous triarylphosphine rhodium complex
IT
     Hydrogenation catalysts
        (preparation of fluorous triarylphosphine rhodium complex as hydrogenation
        catalyst for cyclohexenone)
     94190-73-5, Triphenyl(3,3,4,4,5,5,6,6,7,7,8,8,8-
     tridecafluorooctyl) phosphonium iodide 94190-74-6,
     (3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Heptadecafluorodecyl)triphenylphosph
     onium iodide
                    130567-58-7, (3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12
     ,12-Heneicosafluorododecyl)triphenylphosphonium iodide
```

RL: RCT (Reactant); RACT (Reactant or reagent)

```
(Wittig reaction with bromobenzaldehyde)
IT
    1122-91-4, 4-Bromobenzaldehyde
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (Wittig reaction with fluorous phosphonium salt)
IT
     354137-11-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (equilibration of free phosphine, chloride bridged dimer and
        corresponding monomer)
     930-68-7, 2-Cyclohexen-1-one
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (fluorous triarylphosphine rhodium catalyzed hydrogenation of)
     14694-95-2, Chlorotris(triphenylphosphine)rhodium
TT
     RL: CAT (Catalyst use); USES (Uses)
        (hydrogenation of fluorous diarylalkenylphosphine catalyzed with)
     353525-51-6P 353525-52-7P
IT
                                353525-53-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and phosphination of)
IT
     353525-57-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction with iridium or rhodium complexes)
                                   353525-60-7P
IT
     353525-54-9P
                    353525-55-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reduction of)
IT
     353525-48-1P
                   353525-49-2P
                                   353525-50-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and rhodium catalyzed hydrogenation of)
IT
     354137-10-3P
     RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation as hydrogenation catalyst and equilibration with free phosphine
        and chloride bridged dimer)
     108-94-1P, Cyclohexanone, preparation
                                             353525-56-1P
                                                             353525-58-3P
TT
     353525-59-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
                  12112-67-3, Bis[(\mu-chloro)(1,5-cyclooctadiene)iridium]
TT
     12092-47-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction with fluorous triarylphosphine)
       71
              THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD
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heptadecafluoroundecyl) - (9CI) (CA INDEX NAME)

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AN
DN
     134:366630
     Entered STN: 25 Mar 2001
ED
     Efficient access to perfluoroalkylated aryl compounds by Heck reaction
тT
     Darses, Sylvain; Pucheault, Mathieu; Genet, Jean-Pierre
ΑU
     Laboratoire de Synthese Selective Organique (UMR 7573, CNRS), Ecole
CS
     Nationale Superieure de Chimie de Paris, Paris, 75231, Fr.
SO
     European Journal of Organic Chemistry (2001), (6), 1121-1128
     CODEN: EJOCFK; ISSN: 1434-193X
     Wiley-VCH Verlag GmbH
PB
DT
     Journal
     English
LA
CC
     25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
os
     CASREACT 134:366630
     Efficient introduction of perfluorinated tails onto aromatic rings has been
AB
     achieved by Heck reaction between perfluoroalkenes and arenediazonium
     salts, catalyzed by palladium acetate. Subsequent transition metal
     catalyzed hydrogenation of the double bond afforded a large variety of
     aromatic compds. bearing an affinity for fluorous solvents. Formation of
     perfluoroalkylated phosphine ligands and their use in palladium-catalyzed
     coupling between potassium trifluoro(vinyl)borates and diazonium salts is
     also described, allowing an easy separation and recycling of the catalytic
     system.
ST
     perfluoroalkylated aryl compd prepn; Heck reaction hydrogenation
     perfluoroalkylated aryl compd prepn; coupling reaction perfluoroalkylated
     phosphine catalyst
IT
     Vinylation
        (Heck; preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
IT
     Perfluorocarbons
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (aryl; preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
IT
     Aromatic hydrocarbons, preparation
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (perfluoro; preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
IT
     Hydrogenation
        (preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
IT
     325459-92-5P
     RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
     USES (Uses)
        (cross-coupling reaction of arenediazonium salts with
        organotrifluoroborates)
IT
     13682-77-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cross-coupling reaction of arenediazonium salts with
        organotrifluoroborates)
IT
     2715-43-7P, Ethyl 4-vinylbenzoate
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (cross-coupling reaction of arenediazonium salts with
        organotrifluoroborates)
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TΤ
     340158-00-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     348-06-1
                369-57-3, Benzenediazonium tetrafluoroborate
                                                                456-27-9
     459-44-9, 4-Methylbenzenediazonium tetrafluoroborate
                                                             500-25-4
     591-18-4, 3-Bromoiodobenzene
                                    624-31-7, 4-Iodotoluene
                                                               673-40-5
     1514-50-7, 4-Iodobenzenediazonium tetrafluoroborate
                                                            10448-07-4
     21652-58-4
                  25291-17-2
                               28912-87-0
                                            340157-80-4
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
IT
     195324-88-0P
                    340157-81-5P
                                   340157-82-6P
                                                   340157-83-7P
     340157-84-8P
                    340157-85-9P
                                   340157-86-0P
                                                   340157-88-2P
                                                                  340157-89-3P
     340157-90-6P
                    340157-91-7P 340157-99-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
IT
     106873-83-0P
                    195324-86-8P
                                   195324-87-9P
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     340157-93-9P
                    340157-94-0P
                                   340157-95-1P
                                                   340157-96-2P
                                                                  340157-97-3P
     340157-98-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of perfluoroalkylated aryl compds. by Heck
        reaction/hydrogenation)
RE.CNT
              THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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- IT 195324-88-0P 340157-99-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of perfluoroalkylated aryl compds. by Heck reaction/hydrogenation)

- RN 195324-88-0 HCAPLUS
- CN Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

RN 340157-99-5 HCAPLUS

CN Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-2-methyl- (9CI) (CA INDEX NAME)

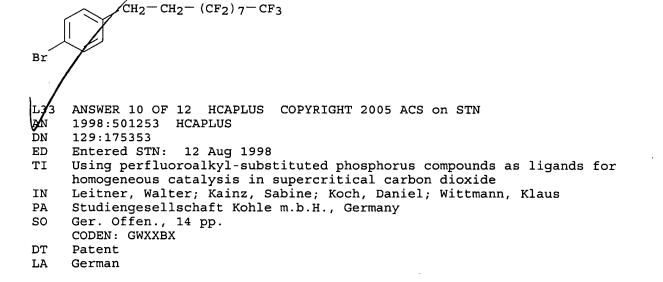
$$\begin{array}{c} \text{CH}_2\text{--}\text{CH}_2\text{---}\left(\text{CF}_2\right)_7\text{---}\text{CF}_3 \\ \text{Me} \end{array}$$

ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN

- AN 2000:859496 HCAPLUS
- DN 134:178294
- ED Entered STN: 08 Dec 2000
- TI Repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system

ΑU Schneider, Siegfried; Bannwarth, Willi Universitat Freiburg Institut fur Chemie und Biochemie, Freiburg, 79104, CS Germany SO Angewandte Chemie, International Edition (2000), 39(22), 4142-4145 CODEN: ACIEF5; ISSN: 1433-7851 PB Wiley-VCH Verlag GmbH Journal DTEnglish LΑ 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds) CC CASREACT 134:178294 OS AΒ Three new perfluoro-tagged Pd complexes, prepared from (4-C8F17C6H4)3P, (3-C8F17C6H4)3P, or (4-C8F17CH2CH2)3P, and Na2[PdCl4], are suitable as catalysts in Stille couplings in a fluorous biphasic system. They can be recycled and reused after phase separation so that they can be applied up to six times without significant reduction in yield. perfluoro palladium catalyst Stille coupling; fluorous biphasic system ST perfluoro palladium catalyst Coupling reaction catalysts IT (Stille; repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system) Solvents IT Stille coupling reaction (repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system) IT 540-80-7 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of) IT 355-02-2, Perfluoromethylcyclohexane 13820-53-6 32875-78-8 RL: RGT (Reagent); RACT (Reactant or reagent) (preparation of) 326475-45-0P 326475-46-1P IT 326475-44-9P RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system) 507-63-1, Perfluorooctyl iodide TΤ 106-37-6, p-Dibromobenzene 580-13-2, 2-Bromonaphthalene 610-94-6, Methyl 4-Iodoaniline 2-bromobenzoate 619-42-1, Methyl 4-bromobenzoate 626-01-7, 2043-53-0 86487-17-4 118486-94-5, Tributyl-2-furyltin 3-Iodoaniline 122439-11-6 RL: RCT (Reactant); RACT (Reactant or reagent) (repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system) IT 195324-88-0P 206560-77-2P 284472-92-0P 325459-90-3P 325459-92-5P 325459-91-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system) 33104-31-3P 39732-01-9P 51792-33-7P 53355-25-2P 63506-58-1P TT 81443-43-8P 89901-00-8P 93321-12-1P 325459-93-6P RL: SPN (Synthetic preparation); PREP (Preparation) (repetitive application of perfluoro-tagged Pd complexes for Stille couplings in a fluorous biphasic system) THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT (1) Betzemeier, B; Angew Chem 1997, V109, P2736 (2) Betzemeier, B; Angew Chem Int Ed Engl 1997, V36, P2623 HCAPLUS (3) Betzemeier, B; Synlett 1999, P489 HCAPLUS (4) Betzemeier, B; Tetrahedron Lett 1998, V39, P6667 HCAPLUS (5) Cornils, B; Angew Chem 1997, V109, P2147 (6) Cornils, B; Angew Chem Int Ed Engl 1997, V36, P2057 HCAPLUS

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IT
     195324-88-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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        couplings in a fluorous biphasic system)
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     heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
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         B01J031-24
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    Section cross-reference(s): 67
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                       C07F009/145+F; C07F009/50A6; C07F009/50A4+F
os
    CASREACT 129:175353; MARPAT 129:175353
    The solubility of P compds. such as those having aryl groups in supercrit. CO2
AB
    is improved by introduction of (CH2)x(CF2)yE groups (E = F \text{ or } H, x = 0-4,
    y = 2-12) so that transition metal complexes of the resulting compds. are
    useful in the catalysis of selective hydrogenation of polyenes to olefins
    and hydroformylation of olefins in supercrit. CO2.
ST
    fluoroalkyl phosphorus compd complex catalyst; supercrit carbon dioxide
    polyene hydrogenation; transition metal complex catalyst polyene
    hydrogenation; olefin hydroformylation transition metal complex catalyst
IT
    Alkenes, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydroformylation; perfluoroalkyl-substituted phosphorus compds. as
       ligands for homogeneous catalysis of reaction of unsatd. compds. in
       supercrit. carbon dioxide)
IT
    Hydroformylation catalysts
        (olefin; perfluoroalkyl-substituted phosphorus compds. as ligands for
       homogeneous catalysis of reaction of unsatd. compds. in supercrit.
       carbon dioxide)
IT
    Supercritical fluids
        (perfluoroalkyl-substituted phosphorus compds. as ligands for
       homogeneous catalysis of reaction of unsatd. compds. in supercrit.
       carbon dioxide)
ΙT
    Transition metal complexes
    RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
    USES (Uses)
       (perfluoroalkyl-substituted phosphorus compds. as ligands for
       homogeneous catalysis of reaction of unsatd. compds. in supercrit.
       carbon dioxide)
IT
    Hydrogenation catalysts
        (polyene; perfluoroalkyl-substituted phosphorus compds. as ligands for
```

homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)

- IT Polyenes
 - RL: RCT (Reactant); RACT (Reactant or reagent)

(selective hydrogenation; perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)

- IT 12279-09-3 32610-47-2
 - RL: RCT (Reactant); RACT (Reactant or reagent) (catalyst precursor; perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)
- IT 111-66-0, 1-Octene
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydroformylation; perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)
- IT 513-35-9P, 2-Methyl-2-butene 563-46-2P, 2-Methyl-1-butene
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (isoprene hydrogenation product; perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)
- IT 195324-85-7P 195324-86-8P 195324-87-9P 195324-88-0P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)

(ligand precursor; perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)

- IT 106-37-6, 1,4-Dibromobenzene 108-36-1, 1,3-Dibromobenzene 109-72-8, Butyllithium, reactions 583-53-9, 1,2-Dibromobenzene 1069-08-5, Diethylaminodichlorophosphine 2043-53-0 2043-57-4, 1H,1H,2H,2H-Perfluorooctyl iodide 7439-95-4, Magnesium, reactions 7719-12-2, Phosphorus trichloride 28240-69-9, 1,2-Bis(dichlorophosphino)ethane
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 (ligand precursor; perfluoroalkyl-substituted phosphorus compds. as
 ligands for homogeneous catalysis of reaction of unsatd. compds. in
 supercrit. carbon dioxide)
- IT 124-19-6P, Nonanal 7786-29-0P, 2-Nonanal
 - RL: IMF (Industrial manufacture); PREP (Preparation) (octene hydroformylation product; perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)
- IT 195324-95-9P 195324-98-2P 195324-99-3P 195325-00-9P 195325-01-0P 195325-02-1P
 - RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)

- IT 195324-89-1P 195324-90-4P 195324-91-5P 195324-92-6P 195324-93-7P 195324-94-8P
 - RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(perfluoroalkyl-substituted phosphorus compds. as ligands for homogeneous catalysis of reaction of unsatd. compds. in supercrit. carbon dioxide)

- IT 124-38-9, Carbon dioxide, uses
 - RL: NUU (Other use, unclassified); USES (Uses)
 (perfluoroalkyl-substituted phosphorus compds. as ligands for
 homogeneous catalysis of reaction of unsatd. compds. in supercrit.
 carbon dioxide)
- IT 78-79-5, Isoprene, reactions

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shiao - 10 / 617431
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (selective hydrogenation; perfluoroalkyl-substituted phosphorus compds.
        as ligands for homogeneous catalysis of reaction of unsatd. compds. in
        supercrit. carbon dioxide)
              THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
       10
RE
(1) Anon; EP 0038701 A2 HCAPLUS
(2) Anon; EP 0155551 A1 HCAPLUS
(3) Anon; JP 05331076 A HCAPLUS
(4) Anon; EP 0614870 A3 HCAPLUS
(5) Anon; EP 0646588 A1 HCAPLUS
(6) Anon; EP 0647647 A1 HCAPLUS
(7) Anon; EP 0684249 A1 HCAPLUS
(8) Anon; US 5171907 HCAPLUS
(9) Anon; US 5382729 HCAPLUS
(10) Anon; Patents Abstracts of Japan 1994, V18(163), PC-1181
     195324-88-0P
     RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
     (Reactant or reagent)
        (ligand precursor; perfluoroalkyl-substituted phosphorus compds. as
        ligands for homogeneous catalysis of reaction of unsatd. compds. in
        supercrit. carbon dioxide)
RN
     195324-88-0 HCAPLUS
     Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
CN
    heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
           CH_2 - CH_2 - (CF_2)_7 - CF_3
    ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
     1997:594034 HCAPLUS
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Br L33 AN DN 127:242400 ED Entered STN: 17 Sep 1997 ΤI Perfluoroalkyl-substituted arylphosphines as ligands for homogeneous catalysis in supercritical carbon dioxide ΑU Kainz, Sabine; Koch, Daniel; Baumann, Wolfgang; Leitner, Walter CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, D-45470, SO Angewandte Chemie, International Edition in English (1997), 36(15), 1628-1630 CODEN: ACIEAY; ISSN: 0570-0833 PB Wiley-VCH DTJournal LΑ English 78-7 (Inorganic Chemicals and Reactions) CC Section cross-reference(s): 29, 67 Perfluoroalkyl-substituted arylphosphine ligands [F(CF2)y(CH2)2-x-AB C6H4] 2PCH2CH2P[C6H4-x-(CH2)2(CF2)yF]2 (3a, x = 2, yr = 6, 3b, x = 3, yr = 6; 3c, x = 4, yr = 6; 3d, x = 4, yr = 8), [F(CF2)6(CH2)2-3-C6H4]3P(4) and [F(CF2)6(CH2)2-4-C6H4]2PCl (5) were prepared Ruthenium and rhodium complexes of 3 and 4, trans-[RuCl2(3c)2], [RhCl(4)3] and [Rh(hfacac)(3)] (hfacac = hexafluoroacetylacetonate), were prepared and the solubility of

[Rh(hfacac)(3)] in supercrit. carbon dioxide (scCO2) was quantified by UV-visible spectroscopy of saturated solns. Rhodium complexes of these

scCO2 compared to their unsubstituted analogs and are thus more suitable for application in homogeneous catalysis. A catalyst formed in situ from

perfluoroalkyl-substituted arylphosphine ligands exhibit enhanced solubility in

[Rh(hfacac)(n4-C8H12)] and 4 catalyzed the hydroformylation of 1-octene in scCO2 to the isomeric aldehydes nonanal and 2-methyloctanal with a 92% conversion and no side reactions. ST rhodium perfluoroalkylarylphosphine complex prepn catalyst soly; arylphosphine perfluoroalkyl rhodium prepn catalyst soly; ruthenium perfluoroalkylarylphosphine complex prepn; phosphine perfluoroalkylaryl rhodium prepn catalyst soly; hydroformylation octene perfluoroalkylarylphosphine rhodium catalyst system; soly supercrit carbon dioxide rhodium perfluoroalkylarylphosphine IT Hydroformylation catalysts (octene hydroformylation in presence of perfluoroalkyl-substituted arylphosphine and rhodium cyclooctadiene hexafluoroacetylacetonato complex catalyst system in supercrit. carbon dioxide) IT Solubility (of rhodium perfluoroalkyl-substituted arylphosphine complexes in supercrit. carbon dioxide) IT 32610-47-2, (η4-(1,5-Cyclooctadiene)) (hexafluoroacetylacetonato) rhodiu RL: CAT (Catalyst use); USES (Uses) (catalytic activity in hydroformylation of octene in supercrit. carbon dioxide) 111-66-0, 1-Octene IT RL: RCT (Reactant); RACT (Reactant or reagent) (catalytic hydroformylation in supercrit. carbon dioxide by perfluoroalkyl-substituted arylphosphine and rhodium cyclooctadiene hexafluoroacetylacetonato complex catalyst system) 1069-08-5, Dichloro (diethylamino) phosphine RL: RCT (Reactant); RACT (Reactant or reagent) (for preparation of perfluoroalkyl-substituted arylphosphine) 195324-93-7P ŦΤ RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (for preparation of rhodium perfluoroalkyl-substituted arylphosphine complex and catalytic activity in hydroformylation of octene in supercrit. carbon dioxide) 108-36-1, 1,3-Dibromobenzene ·IT 583-53-9, 1,2-Dibromobenzene 7719-12-2, Phosphorus chloride (PCl3) RL: RCT (Reactant); RACT (Reactant or reagent) (for preparation of rhodium perfluoroalkyl-substituted arylphosphine complexes) IT 195324-85-7P 195324-86-8P 195324-88-0P 195324-89-1P 195324-90-4P 195324-92-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (for preparation of rhodium perfluoroalkyl-substituted arylphosphine complexes) 106-37-6, 1,4-Dibromobenzene 2043-57-4 28240-69-9, 1,2-Bis (dichlorophosphino) ethane RL: RCT (Reactant); RACT (Reactant or reagent) (for preparation of ruthenium and rhodium perfluoroalkyl-substituted arylphosphine complexes) IT 195324-87-9P 195324-91-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (for preparation of ruthenium and rhodium perfluoroalkyl-substituted arylphosphine complexes) IT 124-38-9, Carbon dioxide, uses RL: NUU (Other use, unclassified); USES (Uses) (perfluoroalkyl-substituted arylphosphines as ligands for homogeneous

195324-99-3P 195325-00-9P 195325-01-0P 195325-02-1P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and solubility in supercrit. carbon dioxide)

catalysis in supercrit. carbon dioxide)

ΙT

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IT
     124-19-6P, Nonanal
                          7786-29-0P, 2-Methyloctanal
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation from catalytic hydroformylation of octene in supercrit. carbon
        dioxide by perfluoroalkyl-substituted arylphosphine and rhodium
        cyclooctadiene hexafluoroacetylacetonato complex catalyst system)
IT
     195324-94-8P
                    195324-95-9P
                                   195324-98-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
IT
     167028-38-8
     RL: PRP (Properties)
        (solubility in supercrit. carbon dioxide)
RE.CNT
              THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Angermund, K; Chem Eur J 1997, V3, P755 HCAPLUS
(2) Burk, M; J Am Chem Soc 1995, V117, P8277 HCAPLUS
(3) Cornils, B; DE 3415968 1984 HCAPLUS
(4) Dinjus, E; Chemistry under Extreme or Non-Classical Conditions 1996, P219
(5) Fornika, R; J Chem Soc Chem Commun 1995, P1479 HCAPLUS
(6) Hadida, S; J Am Chem Soc, in press 1994
(7) Horvath, I; Science 1994, V266, P72 HCAPLUS
(8) Jessop, P; J Am Chem Soc 1996, V118, P344 HCAPLUS
(9) Jessop, P; Science 1995, V269, P1065 HCAPLUS
(10) Kaupp, G; Angew Chem 1994, V106, P1519 HCAPLUS
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(12) Langer, F; Tetrahedron: Asymmetry 1997, V8, P715 HCAPLUS
(13) Morgenstern, D; Green Chemistry, ACS Symp Ser 1996, V626, P132ff
(14) Poliakoff, M; Angew Chem Int Ed Engl 1995, V34, P1275 HCAPLUS
(15) Poliakoff, M; Angew Chem Int Ed Engl 1995, V107, P1409
(16) Rathke, J; US 5198589 1993 HCAPLUS
(17) Rathke, J; Organometallics 1991, V10, P1350 HCAPLUS
(18) Reetz, M; Chimia 1993, V47, P493 HCAPLUS
(19) Xiao, J; Tetrahedron Lett 1996, V37, P2813 HCAPLUS
(20) Zosel, K; Angew Chem 1978, V90, P748 HCAPLUS
(21) Zosel, K; Angew Chem Int Ed Engl 1978, V17, P702
IT
     195324-88-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (for preparation of rhodium perfluoroalkyl-substituted arylphosphine
        complexes)
RN
     195324-88-0 HCAPLUS
CN
     Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
     heptadecafluorodecyl) - (9CI) (CA INDEX NAME)
           CH_2 - CH_2 - (CF_2)_7 - CF_3
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Br
£33
     ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     1992:501039 HCAPLUS
DN
     117:101039
ED
     Entered STN: 05 Sep 1992
TI
     Photoimaging compositions containing 2-diazo-1,2-quinone derivatives
     Wakamatsu, Kan; Wakata, Yuichi; Satomura, Masato; Namiki, Tomizo
IN
     Fuji Photo Film Co., Ltd., Japan
PA
     Eur. Pat. Appl., 16 pp.
so
     CODEN: EPXXDW
DT
     Patent
     English
LA
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IC ICM C07C309-76

ICS C07C245-12; G03F007-004

ECLA

ECLA

G03F007/022

G03F007/022

CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

FAN.CNT 1

PATENT NO.		KIND	DATE	APPLICATION NO.	DATE	
ΡI	EP 468531		A1	19920129	EP 1991-112624	19910726 <
	EP 468531		B1	19941214		
	EP 468531		B2	19971112		
	R: DE,	FR, GB,	IT			
	JP 04089469	•	A2	19920323	JP 1990-400059	19901201 <
	US 5312905		A	19940517	US 1991-736343	19910726 <
	US 5384227		Α	19950124	US 1993-93722	19930720 <
	US 5514518		Α	19960507	US 1994-315574	19940930 <
PRAI	JP 1990-200	989	Α	19900727	<	
	JP 1990-400	059	Α	19901201	<	
	US 1991-736	343	A3	19910726	<	
	US 1993-937	22	A3	19930720	<	
CLASS						
PATE	ENT NO.	CLASS	PATENT	FAMILY CLA	SSIFICATION CODES	
EP 468531 ICM ICS		C07C309-76				
		ICS	C07C245-12; G03F007-004			

C07C309/71; C07C309/76; C07C309/77; C07C323/20;

C07C309/71; C07C309/76; C07C309/77; C07C323/20;

OS MARPAT 117:101039

GΙ

EP 468531

US 5384227

$$N_2$$
 R_1
 R_2
 R_2
 R_1

- AB Photoimaging compns., which are suited for making color proofs, resist patterns, printing plates, and presensitized lithog. plates, comprises a 2-diazo-1,2-quinone derivative having the formula I (one of R1 and R2 is H and the other is a substituent group containing an alkyl group which is substituted by ≥ 1 F atom or the substituent group has the formula SO3R3 or SO2NR4R5 where R3 and ≥ 1 of R4 and R5 represent a substituent group containing an alkyl group having 2-20 C atoms and substituted by ≥ 3 F atoms) and a polymer having a softening temperature $\leq 60^{\circ}$.
- ST photoimaging compn diazoquinone deriv resist; printing plate photosensitive compn diazoquinone; color proofing photosensitive compn diazoquinone
- IT Photoimaging compositions and processes

(containing diazoquinone derivs. and polymers having low softening temperature)

IT Printing plates

(manufacture of, color proofing in, photosensitive compns. containing diazoquinone derivs. and polymers having low softening temperature for)

IT Polyamides, uses

RL: PREP (Preparation)

(photoimaging compns. containing diazoquinone derivs. and, for color

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proofing and lithog. plate preparation)
IT
     Vinyl acetal polymers
     RL: PREP (Preparation)
        (butyrals, photoimaging compns. containing diazoquinone derivs. and, for
        color proofing and lithog. plate preparation)
IT
     Resists
        (photo-, containing diazoquinone derivs. and polymers having low softening
        temperature)
IT
     Lithographic plates
        (presensitized, containing diazoquinone derivs. and polymers having low
        softening temperature)
     100-42-5D, Styrene, copolymers with maleic acid semiesters
IT
                                                                   110-16-7D,
     Maleic acid, semiesters, copolymers with styrene
     RL: USES (Uses)
        (photoimaging compns. containing diazoquinone derivs. and, for color
        proofing and lithog. plate preparation)
IT
     101320-96-1P 142623-70-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, in preparing diazoguinone derivs. for
        photoimaging compns.)
IT
     142623-67-4P
                    142623-68-5P
                                   142623-69-6DP, derivs.
                                                             142623-71-0P
     142623-72-1P
                    142623-73-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and use of, as photosensitive compound in photoimaging compns.)
IT
     142623-70-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, in preparing diazoguinone derivs. for
        photoimaging compns.)
RN
     142623-70-9 HCAPLUS
CN
     Phenol, 4-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-
     heptadecafluorodecyl)thio] - (9CI) (CA INDEX NAME)
           S-CH_2-CH_2-(CF_2)_7-CF_3
     134 all hitstr tot
     ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     2004:991071 HCAPLUS
DN
     142:134436
ED
     Entered STN: 19 Nov 2004
ΤI
     Fluorous Mixture Synthesis of 4-Alkylidene Cyclopentenones via a
     Rhodium-Catalyzed [2+2+1] Cycloaddition of Alkynyl Allenes
ΑU
     Manku, Sukhdev; Curran, Dennis P.
CS
     Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260,
     USA
SO
     Journal of Combinatorial Chemistry (2005), 7(1), 63-68
     CODEN: JCCHFF; ISSN: 1520-4766
     American Chemical Society
PΒ
DT
     Journal
     English
LA
     27-18 (Heterocyclic Compounds (One Hetero Atom))
CC
     CASREACT 142:134436
OS
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GI

II

$$\mathbb{R}^{1}$$
 $\mathbb{M}^{\mathbb{N}}$ \mathbb{R}^{2} \mathbb{R}^{1} $\mathbb{R}^{\mathbb{N}}$ $\mathbb{R}^{\mathbb{N}}$ $\mathbb{R}^{\mathbb{N}}$

A combinatorial library of 16 oxodihydropyrindolecarboxylate AB hydrochlorides I•HCl (R = Me, Ph, BuCH2, Me2CHCH2; R1 = Me, EtCH2, Me2CHCH2, PhCH2) is prepared from amino acids and propargyl bromides using (fluoroalkylethyl)benzyl protecting groups to allow the reaction products to be separated readily by conventional silica gel chromatog. Protection of amino acids with the N-hydroxysuccinimidyl esters of 4-(2fluoroalkylethyl)benzylcarbonic acids yields protected amino acids 4-R2NHCH(R1)CO2H [R1 = Me, PhCH2, EtCH2, Me2CHCH2; R2 = 4-R3CH2CH2C6H4CH2OCO; R3 = F3C(CF2)n, (F3C)2CF(CF2)6; n = 3, 5, 7] ofwhich four are selected for use in the combinatorial library synthesis because of their separability. Esterification of the fluorous protected amino acids with 4-trimethylsilyl-3-butyn-2-ol yields individual fluorous protected amino acid propargyl esters. Claisen rearrangement of zinc enolates of the amino acid esters, methylation of the free acids, desilylation, and alkylation of the amino groups with propargyl bromides yields allenyl amino acids II [R = Me, Ph, BuCH2, Me2CHCH2; R1 = Me, EtCH2, Me2CHCH2, PhCH2; R2 = 4-R3CH2CH2C6H4CH2OCO; R3 = F3C(CF2)n, (F3C)2CF(CF2)6; n = 3, 5, 7] diastereoselectively as mixts. derived from a single propargyl bromide starting material. In the key step, Pauson-Khand cyclocarbonylation of mixts. of II in the presence of bis(chlorodicarbonylrhodium), triphenylphosphine, and silver tetrafluoroborate in dichloroethane at 40° yields oxodihydropyrindolecarboxylates III [R = Me, Ph, BuCH2, Me2CHCH2; R1 = Me, EtCH2, Me2CHCH2, PhCH2; R2 = 4-R3CH2CH2C6H4CH2OCO; R3 = F3C(CF2)n, (F3C)2CF(CF2)6; n = 3, 5, 7]. Cleavage of the fluorous benzylcarbamate protecting groups with di-Me sulfide and boron trifluoride etherate followed by treatment with hydrogen chloride in ether yields the title compds. I.HCl; the deprotection conditions erode the stereoselectivity of the overall reaction significantly, but other methods are not successful at removing the fluorous carbamate protecting groups. ST alkylidene oxodihydropyrindolecarboxylate hydrochloride combinatorial library prepn; protected fluorous propargyl allenyl amino acid stereoselective prepn; fluorous benzylcarbamate protecting group sepn oxodihydropyrindolecarboxylate combinatorial library; stereoselective Pauson Khand reaction allenyl alkyne fluorous protecting group; combinatorial synthesis fluorous protecting group product sepn; rhodium catalyzed Pauson Khand cyclocarbonylation alkynyl allene IT Combinatorial chemistry

Combinatorial library Protective groups

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT Amino acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT Pauson-Khand reaction

Pauson-Khand reaction catalysts

Stereoselective synthesis

(the use of a stereoselective rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step in the preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups)

IT 603-35-0, Triphenylphosphine, uses 14104-20-2, Silver tetrafluoroborate 14523-22-9, Bis(dicarbonylrhodium chloride)

RL: CAT (Catalyst use); USES (Uses)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

825636-09-7P 825636-10-0P 825636-11-1P TT 825636-12-2P 825636-13-3P 825636-14-4P 825636-15-5P 825636-16-6P 825636-17-7P 825636-18-8P 825636-19-9P 825636-20-2P 825636-21-3P 825636-22-4P 825636-23-5P 825636-24-6P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

825635-69-6P 825635-70-9P 825635-71-0P IT 825635-72-1P 825635-73-2P 825635-74-3P 825635-75-4P 825635-76-5P 825635-77-6P 825635-78-7P 825635-79-8P 825635-80-1P 825635-81-2P 825635-82-3P 825635-83-4P 825635-84-5P 825635-85-6P 825635-86-7P 825635-87-8P 825635-88-9P 825635-89-0P 825635-90-3P 825635-91-4P 825635-92-5P 825635-93-6P 825635-94-7P 825635-95-8P 825635-96-9P 825635-97-0P 825635-98-1P 825635-99-2P 825636-00-8P 825636-01-9P 825636-02-0P 825636-03-1P 825636-04-2P 825636-05-3P 825636-06-4P 825636-07-5P 825636-08-6P RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT 1794-48-5, 1-Bromo-3-phenyl-2-propyne 3355-28-0, 1-Bromo-2-butyne 18495-27-7, 1-Bromo-2-octyne 185030-28-8, 1-Bromo-4-methyl-2-pentyne RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT 825635-61-8P 825635-64-1P 825635-65-2P 825635-68-5P RL: CRT (Combinatorial reactant); RCT (Reactant); SPN (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) 61-90-5, Leucine, reactions 56-41-7, Alanine, reactions 63-91-2, Phenylalanine, reactions 6600-40-4, Norvaline 6999-19-5, 556050-48-7 **556050-49-8** 4-(Trimethylsilyl)-3-butyn-2-ol 825635-46-9 825635-47-0 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) 556050-59-0P 825635-48-1P 825635-51-6P 825635-53-8P 825635-54-9P 825635-56-1P 825635-57-2P 825635-60-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) 556050-51-2P 556050-54-5P 825635-49-2P 825635-50-5P 825635-52-7P 825635-55-0P 825635-58-3P 825635-59-4P 825635-62-9P 825635-63-0P 825635-66-3P 825635-67-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD 20 (1) Brummond, K; Org Lett 2002, V4, P1931 HCAPLUS (2) Brummond, K; Org Lett, in press 2004 (3) Corbell, G; The Alkaloids 1977, V16, P432 (4) Curran, D; Handbook of Fluorous Chemistry 2004, P101 (5) Curran, D; J Org Chem 2003, V68, P4643 HCAPLUS (6) Curran, D; Synlett 2001, P1488 HCAPLUS (7) Curran, D; Tetrahedron 2001, V57, P5243 HCAPLUS (8) Dandapani, S; Proc Nat Acad Sci U S A, in press 2002 (9) Greene, T; Protective Groups in Organic Synthesis, 3rd ed 1999 (10) Gunter, M; J Org Chem 2003, V68, P8037 (11) Haggerty, S; Chem Biol 2003, V10, P383 (12) Hammouda, Y; J Pharm Pharmacol 1964, P833 HCAPLUS (13) Kazmaier, U; Synthesis 1996, P1489 HCAPLUS (14) Koehler, A; J Am Chem Soc 2003, V125, P8420 HCAPLUS (15) Luo, Z; J Org Chem 2001, V66, P4261 HCAPLUS (16) Luo, Z; Science 2001, V291, P1766 HCAPLUS (17) Pelish, H; J Am Chem Soc 2001, V123, P6740 HCAPLUS (18) Schreiber, S; Science 2000, V287, P1964 HCAPLUS (19) Zhang, Q; J Am Chem Soc 2004, V126, P36 HCAPLUS (20) Zhang, W; J Am Chem Soc 2002, V124, P10443 HCAPLUS 556050-49-8 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the

556050-49-8 HCAPLUS RN

step)

IT

IT

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RE

IT

2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-CN heptadecafluorodecyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key

L34 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:713708 HCAPLUS

DN 141:366039

ED Entered STN: 01 Sep 2004

TI Stereoisomer libraries: Total synthesis of all 16 stereoisomers of the pine sawfly sex pheromone by a fluorous mixture-synthesis approach

AU Dandapani, Sivaraman; Jeske, Mario; Curran, Dennis P.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO Proceedings of the National Academy of Sciences of the United States of America (2004), 101(33), 12008-12012
CODEN: PNASA6; ISSN: 0027-8424

PB National Academy of Sciences

DT Journal

LA English

CC 26-2 (Biomolecules and Their Synthetic Analogs)

GI

AB All 16 stereoisomers of the sex pheromone of pine sawfly (3,7,11-trimethyltridecyl propanoate) have been synthesized on a 10- to 20-mg scale by a split-parallel fluorous mixture-synthesis approach. Thus, a mixture of (R,R)-, (S,S)-, (S,R)-, and (R,S)-MeCH(OH)CHMeCH2OH was added to Rf(CH2)3OC6H4CHO-4 (Rf = C4F9, C6F13, C8F17, C7F15) to give a mixture consisting of dioxanes I which were subsequently converted to the title

shiao - 10 / 617431 compds. Spectral data obtained for all 32 compds. (16 alcs. and the corresponding propionates) matched well with published data, thereby validating the fluorous-tag encoding of diastereoisomers. This fluorous-tag encoding method is recommended for the efficient synthesis of multiple stereoisomers for spectroscopic studies, biol. tests, or other structure-function relationships. pine sawfly sex pheromone fluorous mixt synthesis; trimethyltridecyl propanoate stereoisomer synthesis; tridecyl propanoate stereoisomer pine sawfly sex pheromone synthesis 86-93-1, 1-Phenyl-1H-tetrazole-5-thiol 79-03-8, Propionyl chloride 87678-97-5, (2R,3S)-2-Methylbutane-1,3-diol 90026-43-0, (2S,3R)-2-Methylbutane-1,3-diol 90026-54-3, (2R,3R)-2-Methylbutane-1,3-116782-41-3, (2S,3S)-2-Methylbutane-1,3-diol 147915-55-7 494798-73-1 780772-19-2 780772-24-9 780772-25-0 780772-26-1 RL: RCT (Reactant); RACT (Reactant or reagent) (total synthesis of all 16 stereoisomers of pine sawfly sex pheromone 3,7,11-trimethyltridecyl propionate using fluorous mixture-synthesis) 250229-78-8P 250229-80-2P 250229-72-2P 333718-17-5P 333718-18-6P 333718-19-7P 333718-20-0P 333718-21-1P 333718-22-2P 333718-23-3P .333718-26-6P 333718-27-7P 333718-24-4P 333718-25-5P 333718-28-8P 333718-29-9P 780772-17-0P 780772-18-1P 780772-20-5P 780772-21-6P 780772-22-7P 780772-23-8P 780772-27-2P 780772-28-3P 780772-29-4P 780772-30-7P 780772-31-8P 780772-32-9P 780772-33-0P 780772-34-1P 780772-35-2P 780772-36-3P 780772-37-4P 780772-38-5P 780772-39-6P 780772-40-9P 780772-41-0P 780772-42-1P 780772-43-2P 780772-44-3P 780772-45-4P 780772-46-5P 780772-49-8P 780772-47-6P 780772-48-7P 780772-50-1P 780772-51-2P 780772-52-3P 780772-53-4P 780772-54-5P 780772-55-6P 780772-56-7P 780772-57-8P 780772-58-9P 780772-59-0P 780772-60-3P 780772-61-4P 780772-62-5P 780772-63-6P 780772-64-7P 780772-69-2P 780772-65-8P 780772-66-9P 780772-67-0P 780772-68-1P 780772-72-7P 780772-73-8P 780772-70-5P 780772-71-6P 780772-74-9P 780772-77-2P 780772-75-0P 780772-76-1P 780772-78-3P 780772-79-4P 780772-80-7P 780772-81-8P 780772-82-9P 780772-83-0P 780772-84-1P 780772-85-2P 780772-86-3P 780772-87-4P 780772-88-5P 780772-89-6P 780772-90-9P 780772-91-0P 780772-92-1P 780772-93-2P 780772-94-3P 780772-95-4P 780772-96-5P 780772-97-6P 780772-98-7P 780772-99-8P 780773-00-4P 780773-01-5P 780773-02-6P 780773-03-7P 780773-04-8P 780773-05-9P 780773-06-0P 780773-07-1P 780773-08-2P 780773-09-3P 780773-10-6P 780773-11-7P 780773-12-8P 780773-13-9P 780773-14-0P 780773-15-1P 780773-16-2P 780773-17-3P 780773-18-4P 780773-19-5P 780773-20-8P 780773-21-9P 780773-22-0P 780773-23-1P 780773-24-2P 780773-25-3P 780773-26-4P 780773-27-5P 780773-28-6P 780773-29-7P

780773-49-1P 780773-51-5P 780773-52-6P 780773-90-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

780773-43-5P

780773-45-7P

780773-47-9P

(total synthesis of all 16 stereoisomers of pine sawfly sex pheromone 3,7,11-trimethyltridecyl propionate using fluorous mixture-synthesis) IT250229-58-4P 250229-59-5P 333718-32-4P 333718-33-5P 333718-34-6P 333718-35-7P 333718-36-8P 333718-37-9P 333718-38-0P 333718-39-1P 333718-42-6P 333718-41-5P 333718-43-7P 333718-40-4P 333718-44-8P 333718-45-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(total synthesis of all 16 stereoisomers of pine sawfly sex pheromone 3,7,11-trimethyltridecyl propionate using fluorous mixture-synthesis)
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) An, H; Chem Rev (Washington, D C) 2000, V100, P3311 HCAPLUS
- (2) Bergstrom, G; Naturwissenschaften 1998, V85, P244

780773-41-3P

- (3) Blakemore, P; J Chem Soc Perkin Trans 1 2002, P2563 HCAPLUS
- (4) Booth, R; J Am Chem Soc 1997, V119, P4882 HCAPLUS
- (5) Curran, D; Org Lett 2002, V4, P2233 HCAPLUS

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780773-39-9P

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(6) Curran, D; Synlett 2001, P1488 HCAPLUS
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- (7) Curran, D; Tetrahedron 2001, V57, P5243 HCAPLUS
- (8) Dandapani, S; Ph D thesis University of Pittsburgh 2004
- (9) Hedenstrom, E; J Chem Ecol 2002, V28, P1237 HCAPLUS
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- (18) Zhang, Q; J Am Chem Soc 2002, V124, P5774 HCAPLUS
- (19) Zhang, Q; J Am Chem Soc 2004, V126, P36 HCAPLUS
- (20) Zhang, W; J Am Chem Soc 2002, V124, P10443 HCAPLUS
- IT 494798-73-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(total synthesis of all 16 stereoisomers of pine sawfly sex pheromone 3,7,11-trimethyltridecyl propionate using fluorous mixture-synthesis)

RN 494798-73-1 HCAPLUS

CN Benzaldehyde, 4-[(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecyl)oxy]- (9CI) (CA INDEX NAME)

1/34 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:683729 HCAPLUS

DN 141:405395

ED Entered STN: 23 Aug 2004

TI New fluorous reversed phase silica gels for HPLC separations of perfluorinated compounds

AU Glatz, H.; Blay, C.; Engelhardt, H.; Bannwarth, W.

CS Institut fuer Organische Chemie und Biochemie, Universitaet Freiburg, Freiburg, 79100, Germany

SO Chromatographia (2004), 59(9/10), 567-570 CODEN: CHRGB7; ISSN: 0009-5893

PB Vieweg Verlag/GWV Fachverlage GmbH

DT Journal

LA English

CC 80-4 (Organic Analytical Chemistry)

AB Two new perfluoroalkyl-modified stationary phases were prepared and compared with two com. available perfluorinated stationary phases (Fluophase RP and Fluophase Pentafluorophenyl) and a C18-RP column with respect to retention times of an array of perfluoroalkyl-tagged and untagged mols. A few highly lipophilic compds. were also included. They showed high retention times on C18-RP columns, but not on perfluorinated support materials. Perfluoroalkyl-tagged compds. revealed a weak interaction with the pentafluorophenyl-modified support. The interaction between perfluoroalkyl-tagged compds. and perfluoroalkyl-modified stationary phases was strong, and dependent on the chain length of the perfluoro tags. Surprisingly, there was only a small difference between the retention times of perfluorinated compds. on C18-RP and C6F13-modified support. Fluorous-fluorous interactions became prevalent only with C8F17-tagged compds. on C8F17 functionalized silica gel. Compds. with two perfluoro tags showed a drastic increase in retention time, which might be due to a cooperative effect. These results demonstrate the uniqueness of

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fluorous-fluorous interactions based on linear perfluoroalkyl chains and open up possibilities for the design of new perfluoro tags for purifications and noncovalent attachments of catalysts or biomols. on perfluorinated solid supports. fluorous reversed phase silica gel HPLC perfluorinated compd sepn HPLC stationary phases (new fluorous reversed phase silica gels for HPLC sepns. of perfluorinated compds.) Perfluoro compounds RL: ANT (Analyte); ANST (Analytical study) (new fluorous reversed phase silica gels for HPLC sepns. of perfluorinated compds.) Silica gel, analysis RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (reaction products, perfluorooctylsilylated or perfluorodecylsilylated; new fluorous reversed phase silica gels for HPLC sepns. of perfluorinated compds.) 50-89-5, Thymidine, analysis 604-32-0, Cholesteryl benzoate 11104-38-4, Vitamin K1 149068-56-4 157829-77-1 163931-45-1 206560-77-2 195324-87-9 **195324-88-0** 195324-86-8 325459-90-3 340157-97-3 785806-72-6 785806-73-7 785806-74-8 785806-75-9 785806-76-0 785806-77-1 RL: ANT (Analyte); ANST (Analytical study) (analyte; new fluorous reversed phase silica gels for HPLC sepns. of perfluorinated compds.) 51851-37-7DP, 1H,1H,2H,2H-Perfluorooctyltriethoxysilane, reaction product with silica gel 101947-16-4DP, 1H, 1H, 2H, 2H-Perfluorodecyltriethoxysilane reaction product with silica gel RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (new fluorous reversed phase silica gels for HPLC sepns. of perfluorinated compds.) 394246-48-1, Fluophase RP 541515-84-8, Fluophase PFP RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); ANST (Analytical study); USES (Uses) (stationary phase for comparison; new fluorous reversed phase silica gels for HPLC sepns. of perfluorinated compds.) RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) Barthelemy, S; Tetrahedron Lett 2002, V43, P807 HCAPLUS (2) Berendsen, G; Anal Chem 1980, V52, P1990 HCAPLUS (3) Berendsen, G; J Liq Chromatogr 1978, V1, P403 HCAPLUS (4) Billiet, H; J Chromatogr 1981, V218, P261 (5) de Miguel, I; Chromatographia 1987, V24, P849 HCAPLUS (6) De Miguel, I; J Chromatogr A 1999, V840, P31 HCAPLUS (7) Dolfinger, R; Anal Chem 2003, V75, P1355 HCAPLUS (8) Endres, A; Chem unserer Zeit 2000, V34, P382 HCAPLUS (9) Engelhardt, H; J Liq Chromatogr 1987, V10, P1999 HCAPLUS (10) Euerby, M; J Sep Sci 2003, V26, P295 HCAPLUS (11) Horvath, I; Science 1994, V266, P72 HCAPLUS (12) Kainz, S; Synthesis 1998, P1425 HCAPLUS (13) Monde, T; J Chromatogr A 1996, V722, P273 HCAPLUS (14) Sadek, P; J Chromatogr 1984, V288, P25 HCAPLUS (15) Schneider, S; Angew Chem Int Ed 2000, V39, P4142 HCAPLUS (16) Schwinn, D; Helv Chim Acta 2003, V86, P188 HCAPLUS (17) Studer, A; Science 1997, V275, P823 HCAPLUS (18) Tzschucke, C; Angew Chem 2002, V114, P4678 195324-88-0 RL: ANT (Analyte); ANST (Analytical study)

(analyte; new fluorous reversed phase silica gels for HPLC sepns. of

perfluorinated compds.)

RN 195324-88-0 HCAPLUS

CN

Benzene, 1-bromo-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

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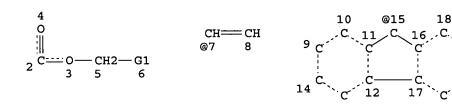
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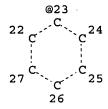
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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

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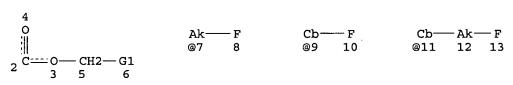
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L36 SCR 1968

L38 35612 SEA FILE=REGISTRY SSS FUL L35 AND L36

L39 STR



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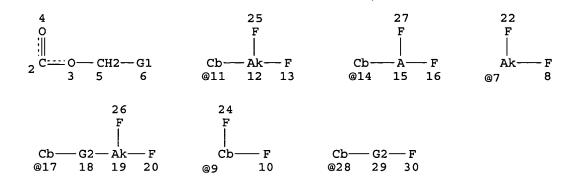
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L42 STI



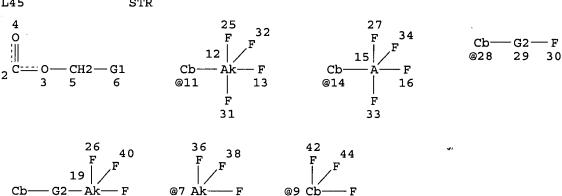
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10

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43

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F

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STEREO ATTRIBUTES: NONE

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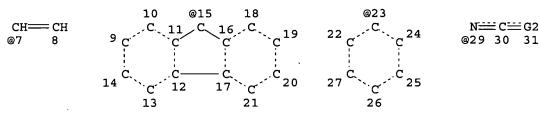
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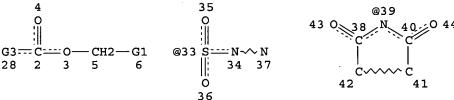
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L50 6 SEA FILE=REGISTRY ABB=ON PLU=ON L49 AND (C18H14F9NO5 OR C20H14F13NO5 OR C23H14F19NO5 OR C22H14F17NO5 OR C29H18F17NO5 OR C13H10F3NO5)

STR





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STEREO ATTRIBUTES: NONE

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C18H8CLF17O2 OR C18H10CLF17O2)

L60 9 SEA FILE=REGISTRY ABB=ON PLU=ON (L50 OR L59)

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L60 9 S L50, L59

SAV TEMP L60 SHIAO617A5/A

L61 7 S L60 NOT L26

FILE 'HCAOLD' ENTERED AT 07:55:25 ON 12 APR 2005

L62 0 S L61

FILE 'HCAPLUS' ENTERED AT 07:55:28 ON 12 APR 2005

L63 6 S L61

L64 1 S L63 AND L1-L12

L65 4 S L63 AND (PD<=20020711 OR PRD<=20020711 OR AD<=20020711)

L66 5 S L64, L65 L67 1 S L63 NOT L66

FILE 'REGISTRY' ENTERED AT 07:56:30 ON 12 APR 2005

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L60 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 825635-47-0 REGISTRY

ED Entered STN: 04 Feb 2005

CN 2,5-Pyrrolidinedione, 1-[[[[4-[3,3,4,4,5,5,6,6,7,7,8,8,9,10,10,10-hexadecafluoro-9-(trifluoromethyl)decyl]phenyl]methoxy]carbonyl]oxy]-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H14 F19 N O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:134436

L60 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 825635-46-9 REGISTRY

ED Entered STN: 04 Feb 2005

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H14 F9 N O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:134436

L60 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 649561-59-1 REGISTRY

ED Entered STN: 12 Feb 2004

CN 2,5-Pyrrolidinedione, 1-[[[[2-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-9H-fluoren-9-yl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C29 H18 F17 N O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:128148

L60 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 556050-49-8 REGISTRY

ED Entered STN: 28 Jul 2003

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H14 F17 N O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:134436

REFERENCE 2: 140:128148

REFERENCE 3: 139:85611

L60 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 556050-48-7 REGISTRY

ED Entered STN: 28 Jul 2003

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H14 F13 N O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:134436

REFERENCE 2: 139:85611

L60 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 495388-43-7 REGISTRY

ED Entered STN: 27 Feb 2003

CN Carbonochloridic acid, [4-[(1E)-3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decenyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H8 Cl F17 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:153811

L60 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 495388-42-6 REGISTRY

ED Entered STN: 27 Feb 2003

CN Carbonochloridic acid, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl)-2-methylphenyl]methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H12 C1 F17 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

$$CH_2-CH_2-(CF_2)_7-CF_3$$
 $C1-C-O-CH_2$
 Me

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:153811

L60 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 495388-41-5 REGISTRY

ED Entered STN: 27 Feb 2003

CN Carbonochloridic acid, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H10 C1 F17 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

$$\begin{array}{c|c} \mathsf{CH}_2-\mathsf{CH}_2-\;(\mathsf{CF}_2)_{\,7}-\mathsf{CF}_3\\ \\ \mathsf{Cl}-\mathsf{C}-\mathsf{O}-\mathsf{CH}_2 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:153811

L60 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN

RN 332378-22-0 REGISTRY

ED Entered STN: 25 Apr 2001

CN 2,5-Pyrrolidinedione, 1-[[[[4-(trifluoromethyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H10 F3 N O5

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:221357

REFERENCE 2: 138:187521

REFERENCE 3: 134:280606

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 07:56:48 ON 12 APR 2005
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FILE COVERS 1907 - 12 Apr 2005 VOL 142 ISS 16 FILE LAST UPDATED: 11 Apr 2005 (20050411/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr tot 166

L66 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:381316 HCAPLUS

DN 139:85611

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ED Entered STN: 20 May 2003
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- TI Synthesis and Reactions of Fluorous Carbobenzyloxy (FCbz) Derivatives of $\alpha\textsc{-Amino Acids}$
- AU Curran, Dennis P.; Amatore, Muriel; Guthrie, David; Campbell, Matthew; Go, Eisan; Luo, Zhiyong
- CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
- SO Journal of Organic Chemistry (2003), 68(12), 4643-4647 CODEN: JOCEAH; ISSN: 0022-3263
- PB American Chemical Society
- DT Journal
- LA English
- CC 34-2 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 6
- OS CASREACT 139:85611
- AB Fluorous carbobenzyloxy (FCbz) reagents Rf(CH2)2-4-C6H4CH2OC(0)OSu (where Su is succinimidoyl and Rf is C6F13 and C8F17) have been used to make FCbz derivs. of 18 of the 20 natural amino acids. The potential utility of this new family of reagents in both standard fluorous synthesis with spe separation
 - and fluorous quasiracemic synthesis is illustrated with representative reactions of the FCbz-Phe derivs.
- ST fluorous carbobenzyloxy prepn amino acid protecting group purifn safety; reagent fluorous carbobenzyloxy prepn amino acid protecting group purifn
- IT Protective groups

Purification

Safety

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

IT Amino acids, preparation

Reagents

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

56-40-6, Glycine, reactions 56-41-7, L-Alanine, reactions TT 56-84-8, h-Asp-oh, reactions 56-85-9, L-Glutamine, L-Serine, reactions 56-86-0, L-Glutamic acid, reactions 56-89-3, Cystine, 60-18-4, L-Tyrosine, reactions 61-90-5, L-Leucine, reactions 63-68-3, h-Met-oh, reactions 63-91-2, L-Phenylalanine, reactions 70-47-3, L-Asparagine, reactions 72-18-4, L-Valine, reactions 73-22-3, h-Trp-oh, reactions L-Threonine, reactions 73-32-5, 108-91-8, Cyclohexanamine, reactions L-Isoleucine, reactions 91-21-4 147-85-3, L-Proline, reactions 153-94-6, D-Tryptophan 312-84-5, D-Serine 319-78-8, D-Isoleucine 328-38-1, D-Leucine 338-69-2, 344-25-2, D-Proline 348-67-4, D-Methionine D-Alanine 349-46-2, 556-02-5, D-Tyrosine 632-20-2, D-Threonine D-Cystine 640-68-6, 673-06-3, D-Phenylalanine 1161-13-3 1783-96-6, D-Aspartic D-Valine 2058-58-4, D-Asparagine 2418-95-3 2740-83-2 3054-01-1 3731-53-1, 4-Pyridinemethanamine 5959-95-5, D-Glutamine 6893-26-1, 31202-69-4 495388-45-9 556050-47-6 D-Glutamic acid RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

- IT 356055-76-0P 356055-77-1P **556050-48-7P** 556050-49-8P
 - 556050-59-0P 556050-78-3P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)
- IT 556050-50-1P 556050-51-2P 556050-52-3P 556050-54-5P 556050-56-7P 556050-58-9P 556050-61-4P 556050-62-5P 556050-64-7P 556050-66-9P 556050-67-0P 556050-68-1P 556050-69-2P 556050-70-5P 556050-71-6P

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556050-74-9P
556050-72-7P
               556050-73-8P
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                                                              556050-76-1P
                               556050-80-7P
                                              556050-81-8P
                                                              556050-82-9P
556050-77-2P
               556050-79-4P
556050-83-0P
                                              556050-86-3P
                                                              556050-87-4P
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556050-98-7P
               556050-99-8P
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                                              556051-01-5P
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RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

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- (2) Curran, D; Angew Chem, Int Ed Engl 1998, V37, P1175 HCAPLUS
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- (11) Rover, S; Tetrahedron Lett 1999, V40, P5667 HCAPLUS
- (12) Studer, A; Science 1997, V275, P823 HCAPLUS
- (13) Wipf, P; Tetrahedron Lett 1999, V40, P4649 HCAPLUS
- (14) Wipf, P; Tetrahedron Lett 1999, V40, P5139 HCAPLUS
- (15) Zhang, Q; J Am Chem Soc 2002, V124, P5774 HCAPLUS
- (16) Zhang, W; J Am Chem Soc 2002, V124, P10443 HCAPLUS
- IT 556050-48-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

RN 556050-48-7 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

- L66 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 2003:196948 HCAPLUS
- DN 138:221357
- ED Entered STN: 12 Mar 2003
- TI Preparation of 2'-aminomethylbiphenyl-2-carboxamides as Kv1.5 potassium

. Page 68

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channel blockers
IN
    Brendel, Joachim; Schmidt, Wolfgang; Below, Peter
    Aventis Pharma Deutschland GmbH, Germany
PA
    U.S., 65 pp., Cont.-in-part of U.S. Ser. No. 675,674.
SO
    CODEN: USXXAM
DT
    Patent
LΑ
    English
IC
    ICM A61K031-44
    ICS C07D213-55; C07D213-56
    514357000; 546264000; 546265000; 546266000; 546267000
NCL
     25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
    Section cross-reference(s): 1, 34
FAN.CNT 3
    PATENT NO.
                       KIND
                              DATE
                                        APPLICATION NO.
                                                                DATE
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    US 6531495
                              20030311 US 2000-698078
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                       B1
                                                                20001030 <--
                                                              19991002 <--
    DE 19947457
                              20010405 DE 1999-19947457
                       Δ1
    US 2003171351
                       A1
                              20030911 US 2002-252385
                                                               20020924 <--
                       B2
                              20040203
    US 6686395
    US 2004102513
                      A1
                              20040527
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PRAI DE 1999-19947457
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                       Α
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                              20000929 <--
    US 2000-675674
    US 2000-698078
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    US 2002-252385
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                              20020924
CLASS
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 US 6531495
                ICM
                      A61K031-44
                ICS
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                       514357000; 546264000; 546265000; 546266000; 546267000
                NCL
                ECLA
                       C07C237/42; C07C335/16; C07D213/40B; C07D233/54C;
 US 6531495
                       C07C271/22; C07C271/54; C07C275/42; C07C311/06;
                       C07C311/13; C07C311/19; C07C311/29; C07C311/46;
                       C07C311/47; C07C317/18
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                ECLA
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                       C07C311/06; C07C311/13; C07C311/19; C07C311/29;
                       C07C311/46; C07C311/47; C07C317/18; C07C335/16;
                       C07D213/40B; C07D233/54C
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 US 2003171351
                ECLA
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                       C07C311/06; C07C311/13; C07C311/19; C07C311/29;
                       C07C311/46; C07C311/47; C07C317/18; C07C335/16;
                       C07D213/40B; C07D233/54C
                                                                         <--
 US 2004102513
                ECLA
                       C07C237/42; C07C271/22; C07C271/54; C07C275/42;
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                       C07C311/46; C07C311/47; C07C317/18; C07C335/16;
                       C07D213/40B; C07D233/54C
                                                                         <--
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    MARPAT 138:221357
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Ι

AΒ Title compds. [I; R1 = CO2R9, SO2R10, COR11, CONR12R13, CSNR12R13; R9, R10, R11, R12 = CmH2mR14; m = 0-4; R14 = (fluoro)alkyl, cycloalkyl, (un) substituted Ph, naphthyl, furyl, etc.; $m \neq 0$ if R14 = (cyclo)alkoxy, SO2Me, or OPh; R2 and R13 = independently H, alkyl, or CF3; R3 = CnH2nR16 or CHR18R19; n = 0-4; $n \neq 0$ if R16 = OR17, SO2Me; R17= H, (cyclo)alkyl, (un)substituted Ph, or pyridyl, R16 = (fluoro)alkyl, cycloalkyl, (un)substituted Ph, naphthyl, furyl, etc.; R18 = H or CpH2pR16; p = 0-3; R19 = CO2H, CONH2, CH2OH, etc.; R4 = H, alkyl, or CF3; or NR3R4 = heterocyclyl; R5, R6, R7, R8 = independently H, halo, CF3, NO2, cyano, etc.; R30 and R31 = independently H or alkyl; CR30R31 = cyclopropyl; and pharmaceutically acceptable salts thereof] were prepared Thus, 2'-aminomethylbiphenyl-2-(N-phenethyl)carboxamide (preparation given) and NaHCO3 in dioxane and H2O were treated dropwise with 4trifluoromethylbenzyl-N-succinimide carbonate (preparation given) in dioxane followed by 12 h stirring at room temperature to give 2'-(4trifluoromethylbenzyloxycarbonylaminomethyl)-biphenyl-2-(Nphenethyl)carboxamide. Tested I inhibited Kv1.5 potassium flow with IC50 = 0.2 µM - 11.3 µM. Thus, I are especially suitable as antiarrhythmic active agents, in particular for the treatment and prophylaxis of atrial arrhythmia, e.g. atrial fibrillation (AF) or atrial flutter (no data). ST aminomethylbiphenylcarboxamide prepn Kv15 potassium channel blocker; biphenylcarboxamide aminomethyl prepn Kv15 potassium channel blocker; heart disease treatment aminomethylbiphenylcarboxamide prepn; antiarrhythmic aminomethylbiphenylcarboxamide prepn , IT Heart, disease

(arrhythmia; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Heart, disease

(atrial fibrillation; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Heart, disease

(atrial flutter; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Ion channel blockers

(potassium; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Antiarrhythmics

Human

Solid phase synthesis

(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Heart, disease

(supraventricular tachycardia; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers)

IT Potassium channel

RL: BSU (Biological study, unclassified); BIOL (Biological study) (voltage-gated, Kv1, blockers; preparation of aminomethylbiphenylcarboxamide

s as Kv1.5 potassium channel blockers) IT Adrenoceptor antagonists (β-, combination therapy; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers) IT RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses) (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT 498577-28-9P RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT 498578-50-0P 498578-51-1P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT 332378-34-4P 332378-35-5P 332378-36-6P 332378-37-7P 332378-38-8P 332378-40-2P 332378-41-3P 332378-42-4P 332378-43-5P 332378-44-6P 332378-45-7P 332378-46-8P 332378-47-9P 332378-48-0P 332378-49-1P 332378-50-4P 332378-51-5P 332378-52-6P 332378-53-7P 332378-54-8P 332378-55-9P 332378-56-0P 332378-57-1P 332378-58-2P 332378-59-3P 332378-60-6P 332378-61-7P 332378-62-8P 332378-63-9P 332378-64-0P 332378-65-1P 332378-66-2P 332378-67-3P 332378-68-4P 332378-69-5P 332378-70-8P 332378-71-9P 332378-72-0P 332378-73-1P 332378-74-2P 332378-75-3P 332378-76-4P 332378-77-5P 332378-78-6P 332378-79-7P 332378-80-0P 332378-81-1P 332378-82-2P 498577-29-0P 498577-30-3P 498577-31-4P 498577-32-5P 498577-33-6P 498577-34-7P 498577-35-8P 498577-36-9P 498577-37-0P 498577-38-1P 498577-39-2P 498577-40-5P 498577-41-6P 498577-42-7P 498577-43-8P 498577-44-9P 498577-45-0P 498577-46-1P 498577-48-3P 498577-49-4P 498577-50-7P 498577-51-8P 498577-53-0P 498577-52-9P 498577-54-1P 498577-55-2P 498577-56-3P 498577-57-4P 498577-58-5P 498577-59-6P 498577-60-9P 498577-61-0P 498577-62-1P 498577-63-2P 498577-64-3P 498577-65-4P 498577-66-5P 498577-67-6P 498577-68-7P 498577-69-8P 498577-70-1P 498577-71-2P 498577-72-3P 498577-73-4P 498577-74-5P 498577-75-6P 498577-76-7P 498577-77-8P 498577-78-9P 498577-79-0P 498577-80-3P 498577-81-4P 498577-82-5P 498577-83-6P 498577-84-7P 498577-85-8P 498577-86-9P 498577-87-0P 498577-88-1P 498577-89-2P 498577-90-5P 498577-91-6P 498577-92-7P 498577-93-8P 498577-94-9P 498577-95-0P 498577-96-1P 498577-97-2P 498577-98-3P 498577-99-4P 498578-00-0P 498578-01-1P 498578-02-2P 498578-03-3P 498578-04-4P 498578-05-5P 498578-06-6P 498578-07-7P 498578-08-8P 498578-09-9P 498578-10-2P 498578-11-3P 498578-12-4P 498578-13-5P 498578-14-6P 498578-15-7P 498578-16-8P 498578-17-9P 498578-18-0P 498578-19-1P 498578-20-4P 498578-21-5P 498578-22-6P 498578-23-7P 498578-24-8P 498578-25-9P 498578-26-0P 498578-27-1P 498578-28-2P 498578-29-3P 498578-30-6P 498578-31-7P 498578-32-8P 498578-33-9P 498578-34-0P 498578-35-1P 498578-36-2P 498578-37-3P 498578-38-4P 498578-39-5P 498578-40-8P 498578-41-9P 498578-42-0P 498578-44-2P 498578-45-3P 498578-46-4P 498578-47-5P 498578-48-6P 498578-49-7P 498578-52-2P 498578-53-3P 498578-55-5P 498578-57-7P 498578-58-8P 498578-59-9P 498578-60-2P 498578-62-4P 498578-63-5P 498578-65-7P 498578-66-8P 498578-68-0P 498578-70-4P 498578-76-0P

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     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5
       potassium channel blockers)
                                                             119297-30-2P
IT
     4445-34-5P, Dibenz[c,e]oxepin-5(7H)-one
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(1) Anon; EP 620216 1994 HCAPLUS
(2) Anon; WO 9625936 1996 HCAPLUS
(3) Anon; WO 9804521 1998 HCAPLUS
(4) Anon; WO 9818475 1998 HCAPLUS
(5) Anon; WO 9818476 1998 HCAPLUS
(6) Anon; CAPLUS 2001:608248 2001
(7) Lullman, H; Pharmakologie und Toxikologie, 1999, P151
(8) Setoi; US 5521170 A 1996 HCAPLUS
(9) Volker, B; Helvetica Chimica Acta 1994, V77, P70
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     Preparation of 2'-aminomethylbiphenyl-2-carboxamides as Kv1.5 potassium
     channel blockers.
    Brendel, Joachim; Schmidt, Wolfgang; Below, Peter
IN
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SO
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OS
     MARPAT 138:187521
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AB Title compds. [I; R1 = CO2R9, SO2R10, COR11, CONR12R13, CSNR12R13; R9, R10, R11, R12 = CmH2mR14; m = 0-4; R14 = (fluoro)alkyl, cycloalkyl, (un) substituted Ph, naphthyl, furyl, etc.; $m \neq 0$ if R14 = (cyclo)alkoxy, SO2Me, or OPh; R2 and R13 = independently H, alkyl, or CF3; R3 = CnH2nR16 or CHR18R19; n = 0-4; $n \neq 0$ if R16 = OR17, SO2Me; R17 = H, (cyclo)alkyl, (un)substituted Ph, or pyridyl, R16 = (fluoro)alkyl, cycloalkyl, (un) substituted Ph, naphthyl, furyl, etc.; R18 = H or CpH2pR16; p = 0-3; R19 = CO2H, CONH2, CH2OH, etc.; R4 = H, alkyl, or CF3; or NR3R4 = heterocyclyl; R5, R6, R7, R8 = independently H, halo, CF3, NO2, cyano, etc.; R30 and R31 = independently H or alkyl; CR30R31 = cyclopropyl; and pharmaceutically acceptable salts thereof] were prepared Thus, 2'-aminomethylbiphenyl-2-(N-phenethyl)carboxamide (preparation given) and NaHCO3 in dioxane and H2O were treated dropwise with 4trifluoromethylbenzyl-N-succinimide carbonate (preparation given) in dioxane followed by 12 h stirring at room temperature to give 2'-(4trifluoromethylbenzyloxycarbonylaminomethyl)-biphenyl-2-(Nphenethyl)carboxamide. Tested I inhibited Kv1.5 potassium flow with IC50 = 0.2 μM - 11.3 μM. Thus, I are especially suitable as antiarrhythmic active agents, in particular for the treatment and prophylaxis of atrial arrhythmia, e.g. atrial fibrillation (AF) or atrial flutter (no data). aminomethylbiphenylcarboxamide prepn Kv15 potassium channel blocker; ST biphenylcarboxamide aminomethyl prepn Kv15 potassium channel blocker; heart disease treatment aminomethylbiphenylcarboxamide prepn; antiarrhythmic aminomethylbiphenylcarboxamide IT

' Heart, disease

(arrhythmia; preparation of aminomethylbiphenylcarboxamides as Kv1.5

potassium channel blockers) IT Heart, disease (atrial fibrillation; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT Heart, disease (atrial flutter; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) Ion channel blockers IT (potassium; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT Antiarrhythmics Solid phase synthesis (preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT Heart, disease (supraventricular tachycardia; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers) IT Potassium channel RL: BSU (Biological study, unclassified); BIOL (Biological study) (voltage-gated, Kv1, blockers; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers) IT Adrenoceptor antagonists $(\beta$ -, combination therapy; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers) IT 332378-39-9P RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses) (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT 498577-28-9P RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) IT 498578-51-1P 498578-50-0P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (antiarrhythmic; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers) 332378-34-4P IT 332378-35-5P 332378-36-6P 332378-37-7P 332378-38-8P 332378-41-3P 332378-42-4P 332378-43-5P 332378-44-6P 332378-40-2P 332378-45-7P 332378-46-8P 332378-47-9P 332378-48-0P 332378-49-1P 332378-51-5P 332378-52-6P 332378-53-7P 332378-54-8P 332378-50-4P 332378-56-0P 332378-57-1P 332378-58-2P 332378-59-3P 332378-55-9P 332378-61-7P 332378-62-8P 332378-63-9P 332378-64-0P 332378-60-6P 332378-65-1P 332378-66-2P 332378-67-3P 332378-68-4P 332378-69-5P 332378-70-8P 332378-71-9P 332378-72-0P 332378-73-1P 332378-74-2P 332378-75-3P 332378-76-4P 332378-77-5P 332378-78-6P 332378-79-7P 332378-80-0P 332378-81-1P 332378-82-2P 498577-29-0P 498577-30-3P 498577-31-4P 498577-32-5P 498577-33-6P 498577-34-7P 498577-35-8P 498577-36-9P 498577-37-0P 498577-38-1P 498577-39-2P 498577-40-5P 498577-41-6P 498577-42-7P 498577-43-8P 498577-44-9P 498577-45-0P 498577-46-1P 498577-48-3P 498577-49-4P 498577-50-7P 498577-51-8P 498577-52-9P 498577-53-0P 498577-54-1P 498577-55-2P 498577-56-3P 498577-57-4P 498577-58-5P 498577-59-6P 498577-60-9P 498577-61-0P 498577-62-1P 498577-63-2P 498577-64-3P 498577-65-4P 498577-66-5P 498577-67-6P 498577-68-7P 498577-69-8P 498577-70-1P 498577-71-2P

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498578-43-1
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(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel

TT

ΙT

blockers)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Brandmeier, V; HELV CHIM ACTA 1994, V77(1), P70 HCAPLUS
- (2) Fujisawa Pharmaceutical Co; EP 0620216 A 1994 HCAPLUS
- (3) Lullman, H; Pharmakologie und Toxikologie 1999, P151
- IT 332378-22-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

RN 332378-22-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(trifluoromethyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

AΒ Three novel fluorinated benzyloxycarbonyl (Cbz) derivs. I-III [R = (CF2)7CF3] were synthesized and used for tagging peptides prepared by Fmoc-based solid-phase approach. The use of a benzyloxycarbonyl-based fluorinated tag facilitated the purification of peptides by fluorous reversed-phase chromatoq.

ST benzyloxycarbonyl fluorophilic prepn peptide tagging reagent chromatog; peptide purifn fluorous reversed phase chromatog

ΙT Solid phase synthesis

(peptide; solid-phase preparation of peptides containing Cbz-based fluorophilic

tagging groups useful for purification by fluorous reversed-phase chromatog.)

IT Purification

(solid-phase preparation of peptides containing Cbz-based fluorophilic tagging

groups useful for purification by fluorous reversed-phase chromatoq.)

TΤ Peptides, preparation

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(solid-phase preparation of peptides containing Cbz-based fluorophilic tagging

groups useful for purification by fluorous reversed-phase chromatoq.) IT 172418-32-5

RL: CAT (Catalyst use); USES (Uses)

(preparation of Cbz-based fluorophilic tagging reagents for purification of synthetic peptides by fluorous reversed-phase chromatog.)

IT 495388-41-5P 495388-42-6P 495388-43-7P

> RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of Cbz-based fluorophilic tagging reagents for purification of synthetic peptides by fluorous reversed-phase chromatoq.)

IT 619-42-1 21652-58-4 99548-55-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of Cbz-based fluorophilic tagging reagents for purification of synthetic peptides by fluorous reversed-phase chromatog.)

IT 495388-45-9P 495388-46-0P 495388-44-8P 495388-47-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of Cbz-based fluorophilic tagging reagents for purification of synthetic peptides by fluorous reversed-phase chromatog.)

495388-50-6P IT 495388-52-8P 495388-53-9P 495388-54-0P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(solid-phase preparation of peptides containing Cbz-based fluorophilic tagging

groups useful for purification by fluorous reversed-phase chromatog.) IT

495388-51-7P 495388-55-1P 495388-56-2P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(solid-phase preparation of peptides containing Cbz-based fluorophilic tagging

groups useful for purification by fluorous reversed-phase chromatog.)
IT 495388-48-2DP, resin-bound 495388-49-3DP, resin-bound 496030-80-9DP,
resin-bound

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(solid-phase preparation of peptides containing Cbz-based fluorophilic tagging

groups useful for purification by fluorous reversed-phase chromatog.)
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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- (2) Ball, H; Int J Peptide Protein Res 1996, V48, P31 HCAPLUS
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- (7) Hancock, W; Anal Biochem 1976, V71, P260 HCAPLUS
- (8) Herrmann, W; Chem Eur J 1997, V3, P1357 HCAPLUS
- (9) Kaiser, E; Anal Biochem 1970, V34, P595 HCAPLUS
- (10) Kent, S; Annu Rev Biochem 1988, V57, P957 HCAPLUS
- (11) Keuning, K; Recl Trav Chim Pays-Bas 1935, V54, P73 HCAPLUS
- (12) Luo, Z; J Org Chem 2001, V66, P4261 HCAPLUS
- (13) Luo, Z; Science 2001, V291, P1766 HCAPLUS
- (14) Merrifield, R; J Am Chem Soc 1963, V85, P2149 HCAPLUS
- (15) Merrifield, R; J Org Chem 1978, V43, P4808 HCAPLUS
- (16) Schwinn, D; Helv Chim Acta 2002, V85, P255 HCAPLUS
- IT 495388-41-5P 495388-42-6P 495388-43-7P

RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of Cbz-based fluorophilic tagging reagents for purification of synthetic peptides by fluorous reversed-phase chromatog.)

RN 495388-41-5 HCAPLUS

CN Carbonochloridic acid, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

RN 495388-42-6 HCAPLUS

CN Carbonochloridic acid, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-2-methylphenyl]methyl ester (9CI) (CA INDEX NAME)

RN 495388-43-7 HCAPLUS

CN Carbonochloridic acid, [4-[(1E)-3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decenyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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(CF<sub>2</sub>) 7
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     ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     2001:239812 HCAPLUS
DN
     134:280606
ED
     Entered STN: 05 Apr 2001
TI
     Preparation of 2'-aminomethylbiphenyl-2-carboxamides as Kv1.5 potassium
     channel blockers.
     Brendel, Joachim; Schmidt, Wolfgang; Below, Peter
IN
PA
     Aventis Pharma Deutschland G.m.b.H., Germany
SO
     Ger. Offen., 28 pp.
     CODEN: GWXXBX
DT
     Patent
LA
     German
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     ICM C07C233-64
     ICS A61K031-166; A61P009-06
     25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
     Section cross-reference(s): 1
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                                DATE
                                            APPLICATION NO.
                                                                    DATE
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CLASS
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PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
DE 19947457	ICM	C07C233-64	
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		C07C311/06; C07C311/13; C07C311/19; C07C311/29; C07C311/46; C07C311/47; C07C317/18; C07C335/16;	
US 6531495	ECLA	C07D213/40B; C07D233/54C C07C237/42; C07C335/16; C07D213/40B; C07D233/54C;	<
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US 2003171351	ECLA	C07C237/42; C07C271/22; C07C271/54; C07C275/42; C07C311/06; C07C311/13; C07C311/19; C07C311/29;	
		C07C311/46; C07C311/47; C07C317/18; C07C335/16; C07D213/40B; C07D233/54C	<
US 2004102513	ECLA	C07C237/42; C07C271/22; C07C271/54; C07C275/42;	
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OS MARPAT 134	. 290606	C07D213/40B; C07D233/54C	<
GI	.200000		

$$R^6$$
 R^5
 $CONR^3R^4$
 R^7

Ι

AΒ Title compds. [I; R1 = CO2R9, SO2R10, COR11, CONR12R13, CSNR12R13; R9, R10, R11, R12 = CmH2mR14; m = 0-4; R14 = (F-substituted) alkyl, cycloalkyl, (substituted) Ph, naphthyl, furyl, etc.; m ≠ 0 if R14 = alkoxy, cycloalkoxy, SO2Me, OCF3; R13 = H, alkyl; R2 = H, alkyl; R3 = CnH2nR16, n = 0-4; $n \neq 0$ if R16 = OR17, SO2Me; R17 = H, alkyl, cycloalkyl, CF3, (substituted) Ph, etc., R16 = (F-substituted) alkyl, cycloalkyl, (substituted) Ph, naphthyl, furyl, etc.; R4 = H, alkyl, etc.; R5, R6, R7, R8 = H, halo, CF3, NO2, cyano, etc.] were prepared Thus, 2'-aminomethylbiphenyl-2-(N-phenethyl)carboxamide (preparation given) and NaHCO3 in dioxane and H2O were treated dropwise with 4trifluoromethylbenzyl-N-succinimide carbonate (preparation given) in dioxane followed by 12 h stirring at room temperature to give 2'-(4trifluoromethylbenzyloxycarbonylaminomethyl)-biphenyl-2-(Nphenethyl)carboxamide. Tested I inhibited Kv1.5 potassium flow with IC50 = $0.3-6.1 \mu M$. β -Blockers and IKs-channel blockers can be used for the tablet formulation. ST aminomethylbiphenylcarboxamide prepn Kv15 potassium channel blocker; biphenylcarboxamide aminomethyl prepn Kv15 potassium channel blocker;

IT Potassium channel
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (Kv1 (potassium channel-forming, voltage-regulated, 1), blockers;

heart disease treatment aminomethylbiphenylcarboxamide prepn;

antiarrhythmic aminomethylbiphenylcarboxamide

preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel
blockers)
Heart, disease
 (atrial fibrillation; preparation of aminomethylbiphenylcarboxamides as
 Kv1.5 potassium channel blockers)
Ion channel blockers

IT Ion channel blockers (potassium; preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Antiarrhythmics

IT

IT

(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT Heart, disease

(supraventricular tachycardia; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers)

IT Adrenoceptor antagonists

 $(\beta$ -, combination therapy; preparation of aminomethylbiphenylcarboxamide s as Kv1.5 potassium channel blockers)

332378-34-4P 332378-35-5P 332378-36-6P 332378-37-7P 332378-38-8P 332378-40-2P 332378-41-3P 332378-42-4P 332378-43-5P 332378-39-9P 332378-45-7P 332378-46-8P 332378-47-9P 332378-48-0P 332378-44-6P 332378-50-4P 332378-51-5P 332378-52-6P 332378-53-7P 332378-49-1P 332378-55-9P 332378-56-0P 332378-57-1P 332378-58-2P 332378-54-8P 332378-59-3P 332378-60-6P 332378-61-7P 332378-62-8P 332378-63-9P 332378-64**-**0P 332378-65-1P 332378-66-2P .332378-67-3P 332378-68-4P 332378-69-5P 332378-70-8P 332378-71-9P 332378-72-0P 332378-73-1P 332378-74-2P 332378-75-3P 332378-76-4P 332378-77-5P 332378-78-6P 332378-79-7P 332378-80-0P 332378-81-1P 332378-82-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

IT 62-53-3, Aniline, reactions 64-04-0, Benzeneethanamine 79-22-1, Methyl chloroformate 98-09-9, Benzenesulfonyl chloride 98-88-4, Benzoyl 103-67-3, Benzylmethylamine 100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions 107-85-7, Isopentylamine 108-91-8, Cyclohexylamine, reactions 111-92-2, Dibutylamine 3-Nitrobenzenesulfonyl chloride 349-88-2, 4-Fluorobenzenesulfonyl 349-95-1, 4-Trifluoromethylbenzyl alcohol 461-18-7, 501-53-1, Benzyl chloroformate 592-34-7, Butyl 4,4,4-Trifluorobutanol chloroformate 701-27-9, 3-Fluorobenzenesulfonyl chloride 2,2,2-Trifluoroethylamine 777-44-6, 3-Trifluoromethylbenzenesulfonyl 1737-26-4 1788-10-9, 4-Acetylbenzenesulfonyl chloride 1885-14-9, Phenyl chloroformate 2706-56-1, 2-(2-Pyridyl)ethylamine 5638-76-6, 2-[2-(Methylaminoethyl)]pyridine 6050-13-1, Diphenic acid 10147-37-2, Isopropylsulfonyl chloride 13139-17-8 16712-69-9, 4-Ethylbenzenesulfonyl chloride 20412-38-8, Neopentyl chloroformate 31140-40-6 39545-31-8 57903-15-8 72235-52-0, 2,4-Difluorobenzylamine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

TΤ 4445-34-5P, Dibenz[c,e]oxepin-5(7H)-one 31638-34-3P 119297-30-2P 332378-21-9P **332378-22-0P** 332378-23-1P 332378-24-2P 332378-25-3P 332378-26-4P 332378-27-5P 332378-28-6P 332378-29-7P 332378-30-0P 332378-31-1P 332378-32-2P 332378-33-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

 potassium channel blockers)

IT 332378-22-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminomethylbiphenylcarboxamides as Kv1.5 potassium channel blockers)

RN 332378-22-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(trifluoromethyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

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     2004:991071 HCAPLUS
AN
DN
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     Entered STN: 19 Nov 2004
ΤI
     Fluorous Mixture Synthesis of 4-Alkylidene Cyclopentenones via a
     Rhodium-Catalyzed [2+2+1] Cycloaddition of Alkynyl Allenes
ΑU
     Manku, Sukhdev; Curran, Dennis P.
CS
     Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260,
so
     Journal of Combinatorial Chemistry (2005), 7(1), 63-68
     CODEN: JCCHFF; ISSN: 1520-4766
PΒ
     American Chemical Society
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     Journal
     English
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os
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A combinatorial library of 16 oxodihydropyrindolecarboxylate AΒ hydrochlorides I • HCl (R = Me, Ph, BuCH2, Me2CHCH2; R1 = Me, EtCH2, Me2CHCH2, PhCH2) is prepared from amino acids and propargyl bromides using (fluoroalkylethyl)benzyl protecting groups to allow the reaction products to be separated readily by conventional silica gel chromatog. Protection of amino acids with the N-hydroxysuccinimidyl esters of 4-(2fluoroalkylethyl)benzylcarbonic acids yields protected amino acids 4-R2NHCH(R1)CO2H [R1 = Me, PhCH2, EtCH2, Me2CHCH2; R2 = 4-R3CH2CH2C6H4CH2OCO; R3 = F3C(CF2)n, (F3C)2CF(CF2)6; n = 3, 5, 7] ofwhich four are selected for use in the combinatorial library synthesis because of their separability. Esterification of the fluorous protected amino acids with 4-trimethylsilyl-3-butyn-2-ol yields individual fluorous protected amino acid propargyl esters. Claisen rearrangement of zinc enolates of the amino acid esters, methylation of the free acids, desilylation, and alkylation of the amino groups with propargyl bromides yields allenyl amino acids II [R = Me, Ph, BuCH2, Me2CHCH2; R1 = Me, EtCH2, Me2CHCH2, PhCH2; R2 = 4-R3CH2CH2C6H4CH2OCO; R3 = F3C(CF2)n, (F3C)2CF(CF2)6; n = 3, 5, 7] diastereoselectively as mixts. derived from a single propargyl bromide starting material. In the key step, Pauson-Khand cyclocarbonylation of mixts. of II in the presence of bis(chlorodicarbonylrhodium), triphenylphosphine, and silver tetrafluoroborate in dichloroethane at 40° yields oxodihydropyrindolecarboxylates III [R = Me, Ph, BuCH2, Me2CHCH2; R1 = Me, EtCH2, Me2CHCH2, PhCH2; R2 = 4-R3CH2CH2C6H4CH2OCO; R3 = F3C(CF2)n, (F3C)2CF(CF2)6; n = 3, 5, 7]. Cleavage of the fluorous benzylcarbamate protecting groups with di-Me sulfide and boron trifluoride etherate followed by treatment with hydrogen chloride in ether yields the title compds. I-HCl; the deprotection conditions erode the stereoselectivity of the overall reaction significantly, but other methods are not successful at removing the fluorous carbamate protecting groups. ST alkylidene oxodihydropyrindolecarboxylate hydrochloride combinatorial library prepn; protected fluorous propargyl allenyl amino acid stereoselective prepn; fluorous benzylcarbamate protecting group sepn oxodihydropyrindolecarboxylate combinatorial library; stereoselective Pauson Khand reaction allenyl alkyne fluorous protecting group; combinatorial synthesis fluorous protecting group product sepn; rhodium catalyzed Pauson Khand cyclocarbonylation alkynyl allene IT

T Combinatorial chemistry Combinatorial library Protective groups (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT Amino acids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT Pauson-Khand reaction

Pauson-Khand reaction catalysts

Stereoselective synthesis

(the use of a stereoselective rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step in the preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups)

IT 603-35-0, Triphenylphosphine, uses 14104-20-2, Silver tetrafluoroborate 14523-22-9, Bis(dicarbonylrhodium chloride)

RL: CAT (Catalyst use); USES (Uses)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT 825636-09-7P 825636-10-0P 825636-11-1P 825636-12-2P 825636-13-3P 825636-14-4P 825636-15-5P 825636-17-7P 825636-16-6P 825636-18-8P 825636-19-9P 825636-20-2P 825636-21-3P 825636-22-4P 825636-23-5P 825636-24-6P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT 825635-69-6P 825635-70-9P 825635-71-0P 825635-72-1P 825635-73-2P 825635-74-3P 825635-75-4P 825635-77-6P 825635-76-5P 825635-78-7P 825635-79-8P 825635-80-1P 825635-81-2P 825635-82-3P 825635-83-4P 825635-84-5P 825635-85-6P 825635-86-7P 825635-87-8P 825635-88-9P 825635-89-0P 825635-90-3P 825635-91-4P 825635-92-5P 825635-93-6P 825635-94-7P 825635-95-8P 825635-96-9P 825635-97-0P 825635-98-1P 825635-99-2P 825636-00-8P 825636-01-9P 825636-02-0P 825636-03-1P 825636-04-2P 825636-05-3P 825636-06-4P 825636-07-5P 825636-08-6P RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT 1794-48-5, 1-Bromo-3-phenyl-2-propyne 3355-28-0, 1-Bromo-2-butyne 18495-27-7, 1-Bromo-2-octyne 185030-28-8, 1-Bromo-4-methyl-2-pentyne RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

IT 825635-61-8P 825635-64-1P 825635-65-2P 825635-68-5P
RL: CRT (Combinatorial reactant); RCT (Reactant); SPN (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the

rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) 56-41-7, Alanine, reactions 61-90-5, Leucine, reactions IT Phenylalanine, reactions 6600-40-4, Norvaline 6999-19-5, 4-(Trimethylsilyl)-3-butyn-2-ol **556050-48-7** 556050-49-8 825635-46-9 825635-47-0 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) IT 556050-59-0P 825635-48-1P 825635-51-6P 825635-53-8P 825635-54-9P 825635-56-1P 825635-57-2P 825635-60-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) IT 556050-51-2P 556050-54-5P 825635-49-2P 825635-50-5P 825635-52-7P 825635-55-0P 825635-58-3P 825635-59-4P 825635-62-9P 825635-63-0P 825635-66-3P 825635-67-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step) RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) Brummond, K; Org Lett 2002, V4, P1931 HCAPLUS (2) Brummond, K; Org Lett, in press 2004 (3) Corbell, G; The Alkaloids 1977, V16, P432 (4) Curran, D; Handbook of Fluorous Chemistry 2004, P101 (5) Curran, D; J Org Chem 2003, V68, P4643 HCAPLUS (6) Curran, D; Synlett 2001, P1488 HCAPLUS (7) Curran, D; Tetrahedron 2001, V57, P5243 HCAPLUS (8) Dandapani, S; Proc Nat Acad Sci U S A, in press 2002 (9) Greene, T; Protective Groups in Organic Synthesis, 3rd ed 1999 (10) Gunter, M; J Org Chem 2003, V68, P8037 (11) Haggerty, S; Chem Biol 2003, V10, P383 (12) Hammouda, Y; J Pharm Pharmacol 1964, P833 HCAPLUS (13) Kazmaier, U; Synthesis 1996, P1489 HCAPLUS (14) Koehler, A; J Am Chem Soc 2003, V125, P8420 HCAPLUS (15) Luo, Z; J Org Chem 2001, V66, P4261 HCAPLUS (16) Luo, Z; Science 2001, V291, P1766 HCAPLUS (17) Pelish, H; J Am Chem Soc 2001, V123, P6740 HCAPLUS (18) Schreiber, S; Science 2000, V287, P1964 HCAPLUS (19) Zhang, Q; J Am Chem Soc 2004, V126, P36 HCAPLUS (20) Zhang, W; J Am Chem Soc 2002, V124, P10443 HCAPLUS 556050-48-7 825635-46-9 825635-47-0 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of a combinatorial library of oxodihydropyrindolecarboxylates using fluorous protecting groups to facilitate separation with the rhodium-catalyzed Pauson-Khand reaction of alkynyl allenes as the key step)

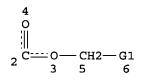
RN 556050-48-7 HCAPLUS

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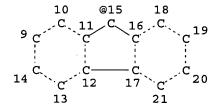
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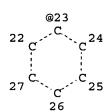
RN 825635-46-9 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,6-nonafluorohexyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

RN 825635-47-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[[4-[3,3,4,4,5,5,6,6,7,7,8,8,9,10,10,10-hexadecafluoro-9-(trifluoromethyl)decyl]phenyl]methoxy]carbonyl]oxy]-(9CI) (CA INDEX NAME)



СН<u> —</u> СН @7 8





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GRAPH ATTRIBUTES:
RSPEC 9 22
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE L36 SCR 1968

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L77 . STR

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L80 1 SEA FILE=REGISTRY ABB=ON PLU=ON L79 AND C32H18CLF39O2SI

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FILE 'HCAPLUS' ENTERED AT 08:08:54 ON 12 APR 2005 L81 2 S L80

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L81 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN MA

2004:57304 HCAPLUS

DN140:127844

ED Entered STN: 23 Jan 2004

Preparation of fluorinated silica gel support material for palladium TI catalyzed coupling reactions

Bannwarth, Willi; Tzschucke, Carl Christoph; Glatz, Heiko; Schwinn, IN Dominik

Albert-Ludwigs-Universitaet Freiburg, Germany PA

SO Ger., 19 pp. CODEN: GWXXAW

DT Patent

LA German

IC ICM C07F007-08 ICS C07B037-00; C07B061-00

21-2 (General Organic Chemistry)

CC Section cross-reference(s): 35, 66

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	WO	2004	0130	68		A1		2004	0212	,	WO 2	003-1	EP75	92		20	00301	714
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			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	·EE,	ES,	FI,	GB,	GD,	GE,	GH,
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PRAI DE 2002-10235225
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CLASS
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DE 10235225
                ICM
                       C07F007-08
                       C07B037-00; C07B061-00
                ICS
                       C07B037/04; C07B043/06; C07B061/00L
DE 10235225
                ECLA
os
    CASREACT 140:127844
AB
    The title support materials were synthesized and their use for palladium
    catalyzed coupling reactions is described. Thus, Rh(PPh3)3Cl-catalyzed
     silylation of HSi(CH2CH2C6F13)3 with triethoxyvinylsilane in THF gave 54%
     (EtO)3SiCH2CH2Si(CH2CH2C6F13)3 which on treatment with activated silica
    gel gave title support material. [(4-F17C8CH2CH2C6H4)3P]2PdCl2-catalyzed
    Suzuki reaction of 4-BrC6H4NO2 with PhB(OH)2 in the presence of above
    prepared fluorinated support material in DME gave quant. yield of
     4-PhC6H4NO2. Also perfluoro-tagged benzyl alc. adsorbed on fluorous
    reversed-phase silica gel derivative via fluorous-fluorous interactions was
    prepared and used in the combinatorial synthesis of quinazolinediones by a
    fluorous biphasic concept without perfluorinated solvents.
ST
    fluorinated silica gel support material prepn catalyst coupling reaction;
    palladium catalyzed Suzuki Sonogashira coupling fluorinated silica gel
    support; cyclization perfluoro tagged benzyl alc carbamate anthanilamide
    quinazolinedione prepn; combinatorial synthesis quinazolinedione
     adsorption fluorous reversed phase silica gel; quinazolinedione synthesis
     combinatorial library; heterocyclization quinazolinedione prepn fluorous
    biphasic concept
IT
    Coupling reaction
     Coupling reaction catalysts
        (Sonogashira; fluorous biphasic catalysis in palladium-mediated Suzuki
       and Sonogashira couplings without perfluorinated solvents)
IT
    Acids, reactions
    Group IIIA element compounds
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (boronic acids, aryl-; fluorous biphasic catalysis in
       palladium-mediated Suzuki and Sonogashira couplings without
       perfluorinated solvents)
TΤ
    Suzuki coupling reaction
     Suzuki coupling reaction catalysts
        (fluorous biphasic catalysis in palladium-mediated Suzuki and
       Sonogashira couplings without perfluorinated solvents)
IT
    Aromatic hydrocarbons, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (halo; fluorous biphasic catalysis in palladium-mediated Suzuki and
       Sonogashira couplings without perfluorinated solvents)
TT
    Combinatorial library
    Polymer-supported reagents
        (preparation of fluorinated silica gel support material for palladium
       catalyzed coupling reactions and perfluoro-tagged benzyl alc. adsorbed
       on fluorous reversed-phase silica gel for combinatorial preparation of
       quinazolinediones)
IT
    Adsorption
    Heterocyclization
        (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
       reversed-phase silica gel derivative via fluorous-fluorous interactions for
```

combinatorial synthesis of quinazolinediones by a fluorous biphasic

concept without perfluorinated solvents)

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ΙT
     Silica gel, preparation
     RL: CAT (Catalyst use); CRG (Combinatorial reagent); RGT (Reagent); SPN
     (Synthetic preparation); CMBI (Combinatorial study); PREP (Preparation);
     RACT (Reactant or reagent); USES (Uses)
        (tridecafluorooctylated; preparation of fluorinated silica gel support for
        palladium catalyzed coupling reactions and perfluoro-tagged benzyl alc.
        adsorbed on fluorous reversed-phase silica gel for preparation of
        quinazolinediones)
     648945-88-4DP, reaction products with silica gel
IT
     RL: CRG (Combinatorial reagent); RGT (Reagent); SPN (Synthetic
     preparation); CMBI (Combinatorial study); PREP (Preparation); RACT
     (Reactant or reagent)
        (FRPSG support; preparation of perfluoro-tagged benzyl alc. adsorbed on
        fluorous reversed-phase silica gel derivative via fluorous-fluorous
        interactions for synthesis of quinazolinediones by a fluorous biphasic
        concept without perfluorinated solvents)
IT
     4441-56-9, Cyclohexylboronic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (attempted; fluorous biphasic catalysis in palladium-mediated Suzuki
        and Sonogashira couplings without perfluorinated solvents)
IT
     326475-46-1
                   343343-17-9
                                 480423-08-3
     RL: CAT (Catalyst use); USES (Uses)
        (fluorous biphasic catalysis in palladium-mediated Suzuki and
        Sonogashira couplings without perfluorinated solvents)
IΤ
     98-80-6, Phenylboronic acid
                                  99-90-1, 1-Acetyl-4-bromobenzene
     4-Bromoanisole
                     348-61-8, 3,4-Difluorobromobenzene
                                                           580-13-2, 2-Naphthyl
     bromide
               586-78-7, 1-Bromo-4-nitrobenzene
                                                 696-62-8, 4-Iodoanisole
     5720-07-0
                 5798-75-4, Ethyl 4-bromobenzoate
                                                    6165-69-1
     3,4,5-Trifluoro-1-bromobenzene
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (fluorous biphasic catalysis in palladium-mediated Suzuki and
        Sonogashira couplings without perfluorinated solvents)
IT
     92-91-1P, p-Acetylbiphenyl
                                 92-93-3P, p-Nitrobiphenyl
     2-Phenylnaphthalene 613-37-6P, p-Methoxybiphenyl
                                                          732-80-9P
                  6301-56-0P, Ethyl biphenyl-4-carboxylate
     2143-90-0P
     28560-79-4P
                   67277-33-2P
                                 172035-84-6P
                                               178820-23-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (fluorous biphasic catalysis in palladium-mediated Suzuki and
        Sonogashira couplings without perfluorinated solvents)
ΙŤ
     51851-37-7DP, reaction products with silica gel
     RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
     USES (Uses)
        (fluorous reversed-phase silica gel (FRPSG) support; preparation of
        fluorinated silica gel support material for palladium catalyzed
        coupling reactions)
TΤ
     14694-95-2, [Chlorotris(triphenylphosphine)]rhodium
     RL: CAT (Catalyst use); USES (Uses)
        (preparation of fluorinated silica gel support material for palladium
        catalyzed coupling reactions)
TT
     78-08-0, Triethoxyvinylsilane
                                     536-74-3, Phenylacetylene
                                                                 147701-73-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of fluorinated silica gel support material for palladium
        catalyzed coupling reactions)
     648945-88-4P
TТ
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of fluorinated silica gel support material for palladium
        catalyzed coupling reactions)
IT
     1942-30-9P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of fluorinated silica gel support material for palladium
        catalyzed coupling reactions)
IT
    1932-42-9P
                 199587-91-2P
                               216311-76-1P 436855-78-6P
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shiao - 10 / 617431
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(Preparation)
   (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
   reversed-phase silica gel derivative via fluorous-fluorous interactions for
   combinatorial synthesis of quinazolinediones by a fluorous biphasic
   concept without perfluorinated solvents)
436855-64-0P
RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT
(Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant
or reagent)
   (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
   reversed-phase silica gel derivative via fluorous-fluorous interactions for
   combinatorial synthesis of quinazolinediones by a fluorous biphasic
   concept without perfluorinated solvents)
89-77-0, 4-Chloroanthranilic acid
                                    100-46-9, Benzylamine, reactions
118-92-3, Anthranilic acid
                            119-68-6, N-Methylanthranilic acid
156-41-2, 2-(4-Chlorophenyl)ethylamine
                                       617-89-0, 2-Furanylmethylamine
                                  501661-50-3, N-(2-
6315-89-5, 3,4-Dimethoxyaniline
Furanylmethyl) anthranilic acid
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial
study); RACT (Reactant or reagent)
   (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
   reversed-phase silica gel derivative via fluorous-fluorous interactions for
   combinatorial synthesis of quinazolinediones by a fluorous biphasic
   concept without perfluorinated solvents)
436855-48-0
RL: CRG (Combinatorial reagent); RGT (Reagent); CMBI (Combinatorial
study); RACT (Reactant or reagent)
   (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
   reversed-phase silica gel derivative via fluorous-fluorous interactions for
   synthesis of quinazolinediones by a fluorous biphasic concept without
   perfluorinated solvents)
503-38-8, Trichloromethyl chloroformate
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial
study); RACT (Reactant or reagent)
   (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
   reversed-phase silica gel derivative via fluorous-fluorous interactions for
   synthesis of quinazolinediones by a fluorous biphasic concept without
   perfluorinated solvents)
436855-64-0P
RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT
(Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant
or reagent)
   (preparation of perfluoro-tagged benzyl alc. adsorbed on fluorous
```

ΤТ

TT

TT

IT

IT

reversed-phase silica gel derivative via fluorous-fluorous interactions for combinatorial synthesis of quinazolinediones by a fluorous biphasic concept without perfluorinated solvents)

RN 436855-64-0 HCAPLUS

Carbonochloridic acid, [4-[tris(3,3,4,4,5,5,6,6,7,7,8,8,8-CN tridecafluorooctyl)silyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

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_ CH2 — O-
                         CH_2 - CH_2 - (CF_2)_5 - CF_3
     ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
     2002:127034 HCAPLUS
DN
     137:32933
ED
     Entered STN: 19 Feb 2002
ΤI
     Perfluoro-tagged benzyloxycarbonyl protecting group and its application in
     fluorous biphasic systems
AU
     Schwinn, Dominik; Bannwarth, Willi
     Institut fur Organische Chemie und Biochemie, Universitat Freiburg,
CS
                                                                       1/1 /- 10 Y
     Freiburg, D-79104, Germany
SO
     Helvetica Chimica Acta (2002), 85(1), 255-264
     CODEN: HCACAV; ISSN: 0018-019X
PΒ
     Verlag Helvetica Chimica Acta
DT
     Journal
LΑ
    -English
CC
     21-2 (General Organic Chemistry)
OS
     CASREACT 137:32933
     The synthesis of a new perfluoro-tagged benzyloxycarbonyl protecting group
AΒ
     is reported, as well as its application in the parallel protection of
     amines. Isolation of the protected amines was performed by simple
     liquid-liquid extraction between perfluorinated and organic solvents.
Deprotection
     was achieved by standard hydrogenolysis. The novel protecting group was also
     applied to cyclization protocols leading to quinazoline-2,4-diones. These
     products were isolated by simple extraction procedures.
     perfluoro tagged benzyloxycarbonyl protecting group prepn; amine perfluoro
     tagged benzyloxycarbonyl protective group; quinazolinedione prepn
     perfluoro tagged benzyloxycarbonyl protective group; fluorous biphasic
     system perfluoro tagged protective group
IT
     Solvents
        (perfluorinated; perfluoro-tagged benzyloxycarbonyl protecting group
        and its application in fluorous biphasic systems)
IT
     Heterocyclization
     Protective groups
        (perfluoro-tagged benzyloxycarbonyl protecting group and its
        application in fluorous biphasic systems)
IT
     Amines, preparation
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (perfluoro-tagged benzyloxycarbonyl protecting group and its
        application in fluorous biphasic systems)
IT
     75-31-0, Isopropylamine, reactions
                                         89-77-0, 4-Chloroanthranilic acid
     118-92-3, Anthranilic acid
                                 333-27-7, Methyl triflate
     Trichloromethyl chloroformate 530-62-1, 1,1'-Carbonyldiimidazole
     873-75-6, 4-Bromobenzyl alcohol
                                       2043-57-4
                                                   3970-21-6
     p-Tolylmagnesium bromide
                                10025-78-2, Trichlorosilane
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (perfluoro-tagged benzyloxycarbonyl protecting group and its
        application in fluorous biphasic systems)
TT
     100-46-9P, Benzylamine, preparation 110-89-4P, Piperidine, preparation
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459-73-4P, Glycine ethyl ester 617-89-0P, Furfurylamine 13360-63-9P,

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Butylethylamine
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                                      147701-73-3P
                                                      201740-57-0P
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     (Reactant or reagent)
        (perfluoro-tagged benzyloxycarbonyl protecting group and its
        application in fluorous biphasic systems)
ΙT
     436855-59-3P
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                                   436855-81-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (perfluoro-tagged benzyloxycarbonyl protecting group and its
        application in fluorous biphasic systems)
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              THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(33) Wu, P; J Chin Chem Soc 2000, V47, P271 HCAPLUS
     436855-64-0P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (perfluoro-tagged benzyloxycarbonyl protecting group and its
        application in fluorous biphasic systems)
RN
     436855-64-0 HCAPLUS
CN
     Carbonochloridic acid, [4-[tris(3,3,4,4,5,5,6,6,7,7,8,8,8-
     tridecafluorooctyl)silyl]phenyl]methyl ester (9CI) (CA INDEX NAME)
```

$$c_{12} - c_{12} - c_{13} - c_{12} - c_{13} - c$$

=> => fil reg FILE 'REGISTRY' ENTERED AT 08:47:53 ON 12 APR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 APR 2005 HIGHEST RN 848290-51-7 DICTIONARY FILE UPDATES: 11 APR 2005 HIGHEST RN 848290-51-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

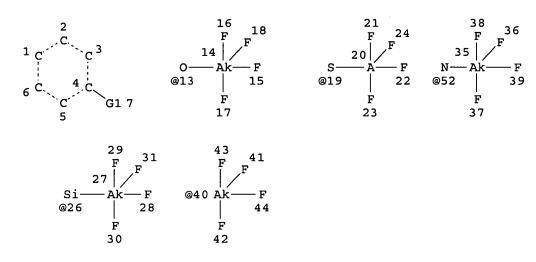
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que 197

L36 SCR 1968 L68 STR



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GRAPH ATTRIBUTES:

RSPEC 4

NUMBER OF NODES IS 36

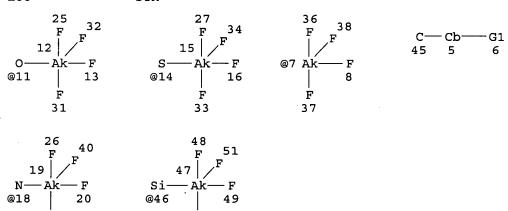
STEREO ATTRIBUTES: NONE

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L72 SCR 1044

L74 37805 SEA FILE=REGISTRY SUB=L70 SSS FUL L68 AND L36 AND L72

L88 STR



VAR G1=7/11/14/18/46
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GGCAT IS MCY UNS AT 9
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

F

39

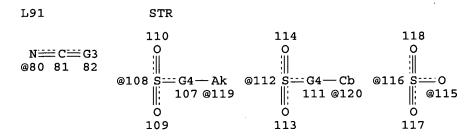
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STEREO ATTRIBUTES: NONE

L89 16283 SEA FILE=REGISTRY SUB=L74 SSS FUL L88

F

50



G2—C—Cb 52 45 5

VAR G2=X/119/108/120/112/116/115/80/SH/OH/NH2
VAR G3=O/S
REP G4=(0-1) O
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

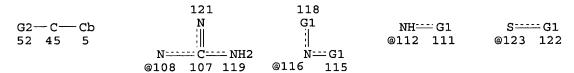
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L93 7961 SE

7961 SEA FILE=REGISTRY SUB=L89 SSS FUL L91

L94 STI



O----- G1 @124 125

VAR G1=AK/CY
VAR G2=108/116/112/123/124
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L96 4820 SEA FILE=REGISTRY SUB=L89 SSS FUL L94

L97 11342 SEA FILE=REGISTRY ABB=ON PLU=ON (L93 OR L96)

=> d his

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                E FLUOROUS/PA,CS
L2
           40 S E3-E16
                E ZHANG W/AU
           1582 S E3-E26
L3
                E ZHANG WEI/AU
           6827 S ZHANG WEI?/AU
L4
                E LUO Z/AU
             63 S E3, E19
L5
                E LUO ZHI/AU
             69 S E3, E32, E86
L6
                E NAGASHIMA T/AU
L7
            168 S E3,E5
                E TADAMICHI/AU
                E CHEN C/AU
L8
           1553 S E3,E18,E22
                E CHEN CHRIS/AU
L9
              7 S E3, E7
L10
             29 S E15-E18
                E YU M/AU
L11
            207 S E3,E24
                E YU MARVIN/AU
L12
             17 S E3-E5
                E SUNGWHAN/AU
                SEL RN L1
     FILE 'REGISTRY' ENTERED AT 06:59:31 ON 12 APR 2005
L13
             84 S E1-E84
L14
              1 S C22H14F17NO5 AND L13
L15
             1 S C18H11F17O2 AND L13
L16
             1 S C29H18F17NO5 AND L13
L17
             1 S C16H8BRF17 AND L13
L18
             2 S C17H10BRF17 AND C6/ES
             0 S C27H14CLF17
L19
L20
             39 S L13 AND F/ELS
L21
             35 S L20 NOT L14-L18
L22
             24 S L21 AND F>=4
L23
             28 S L14-L17, L22
L24
             30 S L18, L23
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L25
              2 S L24
     FILE 'REGISTRY' ENTERED AT 07:08:18 ON 12 APR 2005
L26
             22 S L24 AND NR>=1
              8 S L24 NOT L26
L27
     FILE 'HCAPLUS' ENTERED AT 07:09:29 ON 12 APR 2005
L28
             19 S L26
L29
              5 S L28 AND L1-L12
L30
              4 S L29 AND (FLUOR?(L)TECH?)/PA,CS
L31
              5 S L29, L30
L32
             14 S L28 NOT L31
L33
             12 S L28 AND (PD<=20020711 OR PRD<=20020711 OR AD<=20020711)
L34
              3 S L32 NOT L33
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     FILE 'HCAPLUS' ENTERED AT 07:12:40 ON 12 APR 2005
     FILE 'REGISTRY' ENTERED AT 07:13:23 ON 12 APR 2005
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L35

STR

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E F/ELS
L36
                SCR 1968
L37
             50 S L35 AND L36
L38
          35612 S L35 AND L36 FUL
                SAV TEMP L38 SHIAO617A/A
L39
                STR L35
L40
             50 S L39 SAM SUB=L38
L41
           7096 S L39 FUL SUB=L38
                SAV TEMP L41 SHIAO617A1/A
L42
                STR L39
L43
             50 S L42 SAM SUB=L41
L44
           4708 S L42 FUL SUB=L41
                SAV TEMP L44 SHIAO617A2/A
L45
                STR L42
L46
             50 S L45 SAM SUB=L44
L47
           3542 S L45 FUL SUB=L44
                SAV TEMP L47 SHIAO617A3/A
L48
           3179 S L47 NOT (PMS OR MXS)/CI
L49
             72 S L48 AND NC4/ES
L50
              6 S L49 AND (C18H14F9NO5 OR C20H14F13NO5 OR C23H14F19NO5 OR C22H1
L51
             29 S L48 AND OC4/ES
L52
            291 S L48 AND S/ELS NOT L49-L51
            289 S L52 NOT (CCS/CI OR SQL/FA)
L53
L54
                STR L35
L55
              1 S L54 SAM SUB=L48
L56
              7 S L54 SAM SUB=L38
L57
            130 S L54 FUL SUB=L38
                SAV L57 TEMP SHIAO617A4/A
L58
             23 S L57 AND L41
L59
              3 S L58 AND (C19H12CLF1702 OR C18H8CLF1702 OR C18H10CLF1702)
L60
              9 S L50, L59
                SAV TEMP L60 SHIAO617A5/A
L61
              7 S L60 NOT L26
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L62
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L63
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L64
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L65
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L66
              5 S L64, L65
L67
              1 S L63 NOT L66
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     FILE 'HCAPLUS' ENTERED AT 07:56:48 ON 12 APR 2005
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L68
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L69
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L70
        2012368 S 46.150.18/RID AND F/ELS
L71
             50 S L68 AND L36 SAM SUB=L70
L72
                SCR 1044
L73
             50 S L68 AND L36 AND L72 SAM SUB=L70
L74
          37805 S L68 AND L36 AND L72 FUL SUB=L70
                SAV TEMP L74 SHIAO6A7B/A
L75
            905 S L38 AND SI/ELS NOT (PMS OR CCS)/CI
L76
                STR L39
L77
                STR L76
             12 S L77 FUL SUB=L38
L78
L79
             3 S L78 AND 1/CL
L80
              1 S L79 AND C32H18CLF3902SI
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FILE 'HCAPLUS' ENTERED AT 08:08:54 ON 12 APR 2005
              2 S L80
L81
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                DEL SHIAO6A7B/A
                SAV TEMP L74 SHIAO617B/A
L82
                STR L45
L83
             50 S L82 SAM SUB=L74
L84
          16196 S L82 FUL SUB=L74
                SAV TEMP L84 SHIAO617B2/A
L85
                STR L82
             50 S L85 SAM SUB=L84
L86
L87
                STR L85
L88
                STR L82
L89
          16283 S L88 FUL SUB=L74
                DEL SHIAO617B2/A
                SAV TEMP L89 SHIAO617B2/A
L90
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L91
                STR L87
L92
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L93
           7961 S L91 FUL SUB=L89
                SAV TEMP L93 SHIAO617B3/A
L94
                STR L91
L95
             50 S L94 SAM SUB=L89
           4820 S L94 FUL SUB=L89
L96
                SAV TEMP L96 SHIAO617B4/A
L97
          11342 S L93, L96
L98
                STR
L99
             50 S L98 SAM SUB=L97
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L100
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L101
           2509 S L97
              4 S L1-L12 AND L101
L102
                SEL HIT RN
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L103
           63 S E1-E63
L104
             58 S L103 NOT L26, L61, L80
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           2505 S L101 NOT L102
L106
           2228 S L105 AND (PD<=20020711 OR PRD<=20020711 OR AD<=20020711)
            460 S L106 AND BENZEN?/SC,SX
L107
              0 S L107 AND TAGGING
L108
              0 S L107 AND TAG?
L109
              3 S L107 AND SCAVEN?
L110
                E SCAVEN/CT
                E E19+ALL
L111
           6664 S E2+NT
                E HALOALKYLATION/CT
L112
            504 S E3-E12
                E E3+ALL
L113
            492 S E3+NT
                E COMBINATORIAL/CT
L114
          22605 S E7+OLD, NT, PFT, RT
L115
          37252 S E5+OLD, NT, PFT, RT
                E E5+ALL
L116
          17055 S E6+OLD, NT, PFT, RT
L117
             58 S L106 AND L111-L116
L118
             39 S L117 AND L107
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L119	48	s	L117 AND L112,L113
L120	0	S	L119 AND L111
L121	0	S	L119 AND L114-L116
L122	19	S	L117-L119 AND P/DT
L123	15	S	L122 AND L112, L113

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=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:48:07 ON 12 APR 2005
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FILE COVERS 1907 - 12 Apr 2005 VOL 142 ISS 16 FILE LAST UPDATED: 11 Apr 2005 (20050411/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l102 bib abs hitstr retable tot

L102 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:209841 HCAPLUS

DN 140:218572

- TI Synthesis of trifluorostyrene derivatives as polymer monomers for proton exchange resins
- IN Lu, Long; Hu, Liqing; Zhang, Weixing; Wang, Yi; Li, Wei; He, Yan
- PA Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China
- SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 13 pp. CODEN: CNXXEV

DT Patent

LA Chinese

FAN.CNT 1

PATEN	T NO.	KIND	DATE	APPLICATION NO.	DATE
PI CN 13	49962	Α	20020522	CN 2001-132099	20011102
PRAI CN 20	01-132099		20011102		

OS MARPAT 140:218572

AB The title monomers are trifluorostyrene derivs. having meta-C2-6 perfluoroalkyl or/and meta-(CF2CF)nOCF2CF2SO2F (Rf) (n=1-4) groups and are synthesized by steps of (1) coupling iodobenzene with iodofluoroalkane derivs. in the presence of Cu at 60-120° for 15-40 h; (2) nitrating the intermediate with HNO3/H2SO4 at 30-60° for 15-40 h, (3) reducing with SnC12·2H2O/concentrated HCl at 30-80° for 0.5-2.0 h to m-Rf-aminobenzene, (3) diazotizing at -5° for 1.0-5.0 h, substituting with KI at 45-75° for 0.5-2.0 h to obtain m-Rf-iodobenzene, and (4) coupling the compound with CF2=CFZnBr in the presence of palladium-based catalyst. The monomers can be used for the proton exchange resin for the proton exchange membrane of fuel cells.

IT 664327-26-8DP, sulfonated

RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses) (prepns. of proton exchange resins from trifluorostyrene derivs.

bearing meta-perfluoroalkyl substituents)

RN 664327-26-8 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[[1,1,2,2,3,3,4,4,5,5,6,6-dodecafluoro-6-[3-(trifluoroethenyl)phenyl]hexyl]oxy]-1,1,2,2-tetrafluoro-, polymer with (trifluoroethenyl)benzene and 1-(trifluoroethenyl)-3-(trifluoromethyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 664327-21-3 CMF C16 H4 F20 O3 S

$$\begin{array}{c|c}
O & CF_2 \\
F - S - CF_2 - CF_2 - O - (CF_2)_6 \\
O & C - F_2
\end{array}$$

CM 2

CRN 82907-02-6 CMF C9 H4 F6

CM 3

CRN 447-14-3 CMF C8 H5 F3

IT 540770-39-6P 664327-20-2P 664327-25-7P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(prepns. of trifluorostyrene derivs. bearing meta-perfluoroalkyl substituents as polymer monomers for proton exchange resins)

RN 540770-39-6 HCAPLUS

CN Benzene, 1-(tridecafluorohexyl)-3-(trifluoroethenyl)- (9CI) (CA INDEX NAME)

RN 664327-20-2 HCAPLUS

CN Benzene, 1-(pentafluoroethy1)-3-(trifluoroetheny1)- (9CI) (CA INDEX NAME)

RN 664327-25-7 HCAPLUS

CN Ethanesulfonyl fluoride, 1,1,2,2-tetrafluoro-2-[1,1,2,2-tetrafluoro-2-[3-(trifluoroethenyl)phenyl]ethoxy]- (9CI) (CA INDEX NAME)

IT 664327-21-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepns. of trifluorostyrene derivs. bearing meta-perfluoroalkyl substituents as polymer monomers for proton exchange resins)

RN 664327-21-3 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[[1,1,2,2,3,3,4,4,5,5,6,6-dodecafluoro-6-[3-(trifluoroethenyl)phenyl]hexyl]oxy]-1,1,2,2-tetrafluoro-(9CI) (CA INDEX NAME)

L102 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:60433 HCAPLUS

DN 140:128148

TI A method for preparing new fluorous tagging and scavenging reactants and uses thereof

IN Zhang, Wei; Luo, Zhiyong; Nagashima, Tadamichi
; Chen, Christine Hiu-Tung; Yu, Marvin S.

PA Fluorous Technologies Incorporated, USA

SO PCT Int. Appl., 83 pp. CODEN: PIXXD2

DT Patent

LA FAN.	English CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	WO 2004007407	A2	20040122	WO 2003-US21686	20030711 <
	WO 2004007407	A3	20041125		
	W: CA, JP				
	RW: AT, BE, BG,	CH, CY	, CZ, DE,	DK, EE, ES, FI, FR, GB,	GR, HU, IE,
	IT, LU, MC,	NL, PT	, RO, SE,	SI, SK, TR	
	US 2004073054	A1	20040415	US 2003-617431	20030711 <
PRAI	US 2002-395067P	P	20020711	<	
	US 2002-396952P	P	20020718		, /
	US 2003-442712P	P	20030127		
	US 2003-442762P	P	20030127	•	
	US 2003-442840P	P	20030127		V
os	MARPAT 140:128148				

GI

IT

RN

modul

AB The present invention includes methods and compns. for increasing the fluorous nature of an organic compound, which contains at least one functional group reactive with group X, by reacting it with at least one fluorous compound of formula XCR1R2(C6H5)m[Wp(CH2)nRf]m [wherein X = a leaving group, a nucleophilic group, or an electrophilic group; R1 and R2 = independently H, alkyl, Ph, (C6R5)q(W')q, or (C6H5)m'[Wp'(CH2)n'Rf]m'; m and m' = independently 1-5; n and n' = independently 0-5; p and p' = independently 0 or 1; q = 0-5; W = O, S, NR3, CR4R5, SIR6R7; W' = OR8, SR9, NR10R11, CR12R13R14, or SiR15R16R17; R3, R4, R5, R8-R14 = independently H, alkyl, aryl, benzyl, or (CH2)n''Rf; R6, R7, R15-R17 = independently alkyl, aryl, benzyl, or (CH2)n''Rf; n'' = 0-5; Rf = perfluoroalkyl, a fluorinated either, or a fluorinate amine; with provisos] to produce a fluorous tagged organic compound The increased fluorous nature of the fluorous tagged organic compound may then be used to sep. the fluorous organic compound from untagged reagents, reactants, catalysts, and/or products derived from it. The resultant fluorous tagged organic compound may also be subjected to subsequent chemical transformations, wherein the fluorous nature of the tagged compound is used to increase the ease of separation of the fluorous tagged organic compound from

Ι

untagged reagents, reactants, catalysts, and/or products derived therefrom, after each chemical transformation. The chemical transformations result in a second fluorous tagged organic compound, which may be reduced by removing the fluorous group thereby producing a second organic compound. The second organic compound may be employed as a pharmaceutical compound or intermediate or as a combinatorial library component. For example, reaction of 4-(1H,1H,2H,2H-perfluorodecyl) benzyl alc. with phosgene in anhydrous THF, followed by coupling with N-hydroxysuccinimide dicyclohexylamine salt in chloroform and workup, provided I (82%).

RL: SPN (Synthetic preparation); PREP (Preparation)

(fluorous tagging and scavenging compound; preparation of new fluorous tagging

and scavenging reactants and uses thereof) 556050-49-8 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

RN 649561-67-1 HCAPLUS

CN Benzene, 1-(chlorodiphenylmethyl)-4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

IT 649561-66-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of new fluorous tagging and scavenging reactants and uses thereof)

RN 649561-66-0 HCAPLUS

CN Benzenemethanol, $4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)-<math>\alpha, \alpha$ -diphenyl- (9CI) (CA INDEX NAME)

IT 356055-77-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of new fluorous tagging and scavenging reactants and uses
 thereof)

RN 356055-77-1 HCAPLUS

CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

$$CH_2-CH_2-(CF_2)_7-CF_3$$

L102 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:501591 HCAPLUS

DN 139:37548

TI Preparation of proton exchange fluoropolymers of trifluorostyrenes and application thereof

IN Lu, Long; Hu, Liqing; Zhang, Weixing; Li, Wei; He, Yan; Wang, Yi

PA Shanghai Inst. of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China

SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 15 pp.

CODEN: CNXXEV

DT Patent

LA Chinese

FAN.CNT 1

FAN.CNI I					
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI CN 1346707	Α	20020501	CN 2001-132100	20011102	
CN 1128679	В	20031126			
PRAI CN 2001-132100		20011102			
GI					

AB The fluoropolymers of trifluorostyrenes (the structural formula I, in which Rf1 is H or CyF2y+1, Rf2 is (CF2CF2)nOCF2CF2SO3H, y = 1, 2, 3, 4, 5 or 6, n = 1, 2, 3 or 4, and m:p:q = 39.2-7.2:9.8-1.8:1) useful for preparing proton exchange membrane in fuel cell had a numeric mol. weight 20- 200 x 104, a dispersion coefficient 1.5-4.5, and an ion exchange capacity 1.5-3.5 mmol HSO4+/g (resin). The synthesizing process comprises (I) radical polymerizing of PhCF=CF2, Rf1PhCF=CF2 and Rf2PhCF=CF2 at a mole ratio of 39.2-7.2:9.8-1.8:1 at 30-70° for 40-100 h in the presences of an initiator (such as K2S2O8) and an emulsifying agent (such as n-C12H25NH2Cl), (II) dissolving the obtained polymer in dichloromethane, and allowing the polymer to sulfonate with a sulfonating agent (a mixture of tri-Et phosphate, SO3 and dichloromethane) at 30-60° for 30 min-1.5 h, hydrolyzing of the sulfonated polymer in an 10-50% aqueous solution of a monobasic metal hydroxide at 60-80° for 4-8 h to obtain a monobasic metal ion exchange resin, and (IV) H+ exchanging of the ion exchange resin with a 0.5-10 mol/L H2SO4 solution for 15-30 min to obtain the product. IT 540770-35-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of proton exchange fluoropolymers of trifluorostyrenes and application thereof)

RN 540770-35-2 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[[6-(3-ethenylphenyl)-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl]oxy]-1,1,2,2-tetrafluoro- (9CI) (CA INDEX NAME)

IT 540770-36-3P 540770-38-5P 540770-40-9P 540770-41-0P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of proton exchange fluoropolymers of trifluorostyrenes and application thereof)

RN 540770-36-3 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[[6-(3-ethenylphenyl)-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl]oxy]-1,1,2,2-tetrafluoro-, polymer with (trifluoroethenyl)benzene and 1-(trifluoroethenyl)-3-(trifluoromethyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-35-2 CMF C16 H7 F17 O3 S

$$F = S - CF_2 - CF_2 - O - (CF_2)_6$$

$$O$$

$$CH = CH_2$$

CM 2

CRN 82907-02-6 CMF C9 H4 F6

CM 3

CRN 447-14-3 CMF C8 H5 F3

RN 540770-38-5 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[2-(3-ethenylphenyl)-1,1,2,2-tetrafluoroethoxy]1,1,2,2-tetrafluoro-, polymer with (trifluoroethenyl)benzene and
1-(trifluoroethenyl)-3-(trifluoromethyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-37-4 CMF C12 H7 F9 O3 S

CM 2

CRN 82907-02-6 CMF C9 H4 F6

CM 3

CRN 447-14-3 CMF C8 H5 F3

RN 540770-40-9 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[[6-(3-ethenylphenyl)-1,1,2,2,3,3,4,4,5,5,6,6dodecafluorohexyl]oxy]-1,1,2,2-tetrafluoro-, polymer with
1-(tridecafluorohexyl)-3-(trifluoroethenyl)benzene and
(trifluoroethenyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-39-6 CMF C14 H4 F16

CRN 540770-35-2 CMF C16 H7 F17 O3 S

CM 3

CRN 447-14-3 CMF C8 H5 F3

RN 540770-41-0 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[2-(3-ethenylphenyl)-1,1,2,2-tetrafluoroethoxy]1,1,2,2-tetrafluoro-, polymer with 1-(tridecafluorohexyl)-3(trifluoroethenyl)benzene and (trifluoroethenyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-39-6 CMF C14 H4 F16

CM 2

CRN 540770-37-4 CMF C12 H7 F9 O3 S

$$_{\text{H}_2\text{C}} = \text{CH}$$
 $_{\text{CF}_2-\text{CF}_2-\text{O}-\text{CF}_2-\text{CF}_2-\text{S}-\text{F}}$
 $_{\text{O}}$

CRN 447-14-3 CMF C8 H5 F3

IT 540770-36-3DP, sulfonated product 540770-38-5DP, sulfonated product 540770-40-9DP, sulfonated product 540770-41-0DP, sulfonated product

RL: PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of proton exchange fluoropolymers of trifluorostyrenes and application thereof)

RN 540770-36-3 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[[6-(3-ethenylphenyl)-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl] 21,1,2,2-tetrafluoro-, polymer with (trifluoroethenyl)benzene and '1-(trifluoroethenyl)-3-(trifluoromethyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-35-2 CMF C16 H7 F17 O3 S

$$\begin{array}{c}
0 \\
F-S-CF_2-CF_2-O-(CF_2)_6 \\
0
\end{array}$$
CH=CH₂

CM 2

CRN 82907-02-6 CMF C9 H4 F6

CRN 447-14-3 CMF C8 H5 F3

RN 540770-38-5 HCAPLUS

CN Ethanesulfonyl fluoride, 2-[2-(3-ethenylphenyl)-1,1,2,2-tetrafluoroethoxy]-1,1,2,2-tetrafluoro-, polymer with (trifluoroethenyl)benzene and 1-(trifluoroethenyl)-3-(trifluoromethyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-37-4 CMF C12 H7 F9 O3 S

$$\begin{array}{c} \text{CF}_2 - \text{CF}_2 - \text{O} - \text{CF}_2 - \text{CF}_2 - \text{S} - \text{F}_1 \\ \text{CF}_2 - \text{CF}_2 - \text{O} - \text{CF}_2 - \text{CF}_2 - \text{S} - \text{F}_2 \\ \text{O} \end{array}$$

CM 2

CRN 82907-02-6 CMF C9 H4 F6

CM 3

CRN 447-14-3 CMF C8 H5 F3

RN 540770-40-9 HCAPLUS
CN Ethanesulfonyl fluoride, 2-[[6-(3-ethenylphenyl)-1,1,2,2,3,3,4,4,5,5,6,6-dodecafluorohexyl]oxy]-1,1,2,2-tetrafluoro-, polymer with 1-(tridecafluorohexyl)-3-(trifluoroethenyl)benzene and (trifluoroethenyl)benzene (9CI) (CA INDEX NAME)

CRN 540770-39-6 CMF C14 H4 F16

CM 2

CRN 540770-35-2 CMF C16 H7 F17 O3 S

$$F = S - CF_2 - CF_2 - O - (CF_2) 6$$

$$O$$

$$CH = CH_2$$

CM 3

CRN 447-14-3 CMF C8 H5 F3

RN 540770-41-0 HCAPLUS

Ethanesulfonyl fluoride, 2-[2-(3-ethenylphenyl)-1,1,2,2-tetrafluoroethoxy]1,1,2,2-tetrafluoro-, polymer with 1-(tridecafluorohexyl)-3(trifluoroethenyl)benzene and (trifluoroethenyl)benzene (9CI) (CA INDEX NAME)

CM 1

CRN 540770-39-6 CMF C14 H4 F16

CM 2

CRN 540770-37-4 CMF C12 H7 F9 O3 S

$$H_2C = CH$$
 $CF_2 - CF_2 - O - CF_2 - CF_2 - S - F$
 $CF_2 - CF_2 - O - CF_2 - CF_2 - S - F$

CM 3

CRN 447-14-3 CMF C8 H5 F3

L102 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:381316 HCAPLUS

DN 139:85611

TI Synthesis and Reactions of Fluorous Carbobenzyloxy (FCbz) Derivatives of $\alpha\textsc{-Amino}$ Acids

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PB American Chemical Society

DT Journal

LA English

OS CASREACT 139:85611

AB Fluorous carbobenzyloxy (FCbz) reagents Rf(CH2)2-4-C6H4CH2OC(0)OSu (where Su is succinimidoyl and Rf is C6F13 and C8F17) have been used to make FCbz derivs. of 18 of the 20 natural amino acids. The potential utility of this new family of reagents in both standard fluorous synthesis with spe separation

and fluorous quasiracemic synthesis is illustrated with representative reactions of the FCbz-Phe derivs.

IT 495388-45-9 556050-47-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

RN 495388-45-9 HCAPLUS

CN Benzoic acid, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{(CF}_2)}_7\text{-}\text{CF}_3\\ \\ \text{MeO-C}\\ \\ \\ \text{O} \end{array}$$

RN 556050-47-6 HCAPLUS

CN Benzoic acid, 4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{CH_2-CH_2-} \left(\operatorname{CF_2}\right) \, 5 - \operatorname{CF_3} \\ \\ \operatorname{MeO-C} \\ \\ \\ \operatorname{O} \end{array}$$

IT 356055-76-0P 356055-77-1P 556050-48-7P

556050-49-8P 556050-59-0P 556050-78-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

RN 356055-76-0 HCAPLUS

CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)- (9CI) (CA INDEX NAME)

$$CH_2-CH_2-(CF_2)_5-CF_3$$

RN 356055-77-1 HCAPLUS

CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)- (9CI) (CA INDEX NAME)

$$_{\rm HO-CH_2}^{\rm CH_2-CH_2-(CF_2)}{_{7}^{-}}{_{\rm CF_3}}$$

RN 556050-48-7 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

RN 556050-49-8 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]oxy]- (9CI) (CA INDEX NAME)

RN 556050-59-0 HCAPLUS

CN L-Phenylalanine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-78-3 HCAPLUS

CN D-Phenylalanine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-

tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 556050-50-1P 556050-51-2P 556050-52-3P 556050-54-5P 556050-56-7P 556050-58-9P 556050-61-4P 556050-62-5P 556050-64-7P 556050-66-9P 556050-67-0P 556050-68-1P 556050-69-2P 556050-70-5P 556050-71-6P 556050-72-7P 556050-73-8P 556050-74-9P 556050-75-0P 556050-76-1P 556050-77-2P 556050-79-4P 556050-80-7P 556050-81-8P 556050-82-9P 556050-83-0P 556050-84-1P 556050-85-2P 556050-86-3P 556050-87-4P 556050-88-5P 556050-89-6P 556050-90-9P 556050-91-0P 556050-92-1P 556050-93-2P 556050-94-3P 556050-95-4P 556050-96-5P 556050-97-6P 556050-98-7P 556050-99-8P 556051-00-4P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and use of fluorous carbobenzyloxy reagents for use in amino acid chemical)

RN556050-50-1 HCAPLUS

CN Glycine, N-[[{4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

RN556050-51-2 HCAPLUS

CN L-Alanine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$HO_2C$$
 S
 N
 O
 CF_3
 CF_3

RN556050-52-3 HCAPLUS

CN L-Valine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10heptadecafluorodecyl)phenyl]methoxy]carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-54-5 HCAPLUS

CN L-Leucine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 556050-56-7 HCAPLUS

CN L-Isoleucine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-58-9 HCAPLUS

CN L-Serine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-61-4 HCAPLUS

CN L-Asparagine, N2-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$H_2N$$
 CF_3
 CF_3
 CF_3

RN 556050-62-5 HCAPLUS

CN L-Glutamine, N2-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 H_2N
 CC_2H
 CC_3
 CC_3

RN 556050-64-7 HCAPLUS

CN L-Threonine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$\begin{array}{c|c} \text{OH} & \text{CF}_2 \end{array} \\ \text{Me} & \begin{array}{c} \text{N} \\ \text{CO}_2 \text{H} & \text{O} \end{array}$$

RN 556050-66-9 HCAPLUS

CN L-Methionine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

MeS
$$S$$
 N O CF_3 CF_3

RN 556050-67-0 HCAPLUS

CN L-Aspartic acid, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$HO_2C$$
 S
 N
 CF_3
 CF_3

RN 556050-68-1 HCAPLUS

CN L-Glutamic acid, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$HO_2C$$
 S
 N
 CO_2H
 O
 CO_2H
 O

RN 556050-69-2 HCAPLUS

CN L-Tryptophan, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 556050-70-5 HCAPLUS

CN L-Tyrosine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$F_3C$$
 (CF2) 7

RN 556050-71-6 HCAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 1-[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10,10-heptadecafluorodecyl)phenyl]methyl] ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 556050-72-7 HCAPLUS

CN Glycine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]metho xy]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{(CF}_2)} \\ & \text{O} \\ & \text{HO}_2\text{C}\text{--}\text{CH}_2\text{--}\text{NH}\text{--}\text{C}\text{--}\text{O}\text{--}\text{CH}_2 \end{array}$$

RN 556050-73-8 HCAPLUS

CN D-Alanine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]met hoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-74-9 HCAPLUS

CN D-Valine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]meth oxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 556050-75-0 HCAPLUS

CN D-Leucine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]met
hoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-76-1 HCAPLUS

CN L-Isoleucine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 556050-77-2 HCAPLUS

Absolute stereochemistry. Rotation (-).

HO
$$R$$
 N O CF_3 CF_3

RN 556050-79-4 HCAPLUS

CN D-Asparagine, N2-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$H_2N$$
 CF_3
 CF_3
 CF_3

RN 556050-80-7 HCAPLUS

CN D-Glutamine, N2-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-81-8 HCAPLUS

CN D-Threonine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 556050-82-9 HCAPLUS

CN D-Methionine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

MeS
$$R$$
 N O CF_3 CF_3

RN 556050-83-0 HCAPLUS

CN D-Aspartic acid, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-84-1 HCAPLUS

CN D-Glutamic acid, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-85-2 HCAPLUS

CN D-Tryptophan, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-86-3 HCAPLUS

CN D-Tyrosine, N-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$F_3C$$
 (CF2) 5

RN 556050-87-4 HCAPLUS

CN 1,2-Pyrrolidinedicarboxylic acid, 1-[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methyl] ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 556050-88-5 HCAPLUS

CN L-Cystine, N,N'-bis[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-

heptadecafluorodecyl)phenyl]methoxy]carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

$$F_3C$$
 (CF2) 7

PAGE 1-B

RN 556050-89-6 HCAPLUS

CN D-Cystine, N,N'-bis[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A

$$F_3C$$
 (CF₂) 5 CO_2H $CO_$

PAGE 1-B

RN 556050-90-9 HCAPLUS

Absolute stereochemistry.

RN 556050-91-0 HCAPLUS

CN L-Lysine, N6-[(1,1-dimethylethoxy)carbonyl]-N2-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heptadecafluorodecyl)phenyl]methoxy]carbonyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-92-1 HCAPLUS

CN D-Lysine, N6-[(1,1-dimethylethoxy)carbonyl]-N2-[[[4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methoxy]carbonyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-93-2 HCAPLUS

CN Carbamic acid, [(1S)-2-(3,4-dihydro-2(1H)-isoquinolinyl)-2-oxo-1-(phenylmethyl)ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-94-3 HCAPLUS

CN Carbamic acid, [(1R)-2-(3,4-dihydro-2(1H)-isoquinoliny1)-2-oxo-1-(phenylmethyl)ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-95-4 HCAPLUS

CN Carbamic acid, [(1S)-2-(cyclohexylamino)-2-oxo-1-(phenylmethyl)ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methy l ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-96-5 HCAPLUS

CN Carbamic acid, [(1R)-2-(cyclohexylamino)-2-oxo-1-(phenylmethyl)ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-97-6 HCAPLUS

CN Carbamic acid, [(1S)-2-oxo-1-(phenylmethyl)-2-[(4-pyridinylmethyl)amino]ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-98-7 HCAPLUS

CN Carbamic acid, [(1R)-2-oxo-1-(phenylmethyl)-2-[(4-pyridinylmethyl)amino]ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 556050-99-8 HCAPLUS

CN Carbamic acid, [(1S)-2-oxo-1-(phenylmethyl)-2-[[[3-(trifluoromethyl)phenyl]methyl]amino]ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)phenyl]methylester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$_{\mathrm{F_{3}C}}$$
 $_{\mathrm{N}}$
 $_{\mathrm{N}}$
 $_{\mathrm{N}}$
 $_{\mathrm{N}}$
 $_{\mathrm{N}}$
 $_{\mathrm{CF_{2})}}$
 $_{\mathrm{7}}$
 $_{\mathrm{CF_{3}}}$

RN 556051-00-4 HCAPLUS

CN Carbamic acid, [(1R)-2-oxo-1-(phenylmethyl)-2-[[[3-(trifluoromethyl)phenyl]methyl]amino]ethyl]-, [4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)phenyl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$_{\mathrm{F_{3}C}}$$

H

R

N

R

H

(CF2) $_{5}$

CF3

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\sim	н.	. 77	ж		м.

Referenced Author	Year	VOL	PG	Referenced Work	Referenced
(RAU)	(RPY)	(RVL)	(RPG)	(RWK)	File
=======================================	+=====	+=====	+=====	+=====================================	+========
Anon				www.fluorous.com	
Curran, D	1998	37	1175	Angew Chem, Int Ed E	HCAPLUS
Curran, D	1999	121	9069	J Am Chem Soc	HCAPLUS
Curran, D	2000			Stimulating Concepts	
Curran, D	2001		1488	Synlett	HCAPLUS
Curran, D	2001	57	5243	Tetrahedron	HCAPLUS
Filippov, D	2002	43	7809	Tetrahedron Lett	HCAPLUS
Green, T	1999		531	Protective Groups in	
Luo, Z	2001	66	4261	J Org Chem	HCAPLUS
Luo, Z	2001	291	1766	Science	HCAPLUS
Rover, S	1999	40	5667	Tetrahedron Lett	HCAPLUS
Studer, A	1997	275	823	Science	HCAPLUS
Wipf, P	1999	40	4649	Tetrahedron Lett	HCAPLUS
Wipf, P	1999	40	5139	Tetrahedron Lett	HCAPLUS
Zhang, Q	2002	124	5774	J Am Chem Soc	HCAPLUS
Zhang, W	2002	124	10443	J Am Chem Soc	HCAPLUS

=> => d l123 bib abs hitstr retable tot

L123 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:115092 HCAPLUS

DN 134:147996

- TI Bis(4-hydroxy-3-perfluoroalkylphenyl)fluoroalkane derivatives and process for the preparation thereof
- IN Adachi, Kenji; Ishihara, Sumi; Oishi, Satoshi; Moriya, Tsukasa

PA Daikin Industries, Ltd., Japan

SO PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010805 W: US	A1	20010215	WO 2000-JP4866	20000721 <
	RW: AT, BE, CH, PT, SE	CY, DE	, DK, ES,	FI, FR, GB, GR, IE, IT,	LU, MC, NL,
	JP 2001048820	A2	20010220	JP 1999-220508	19990803 <
PRAI	JP 1999-220508	Α	19990803	<	
OS GT	MARPAT 134:147996				

AB Bis(4-hydroxy-3-perfluoroalkylphenyl)fluoroalkane derivs. represented by general formula I are provided, wherein R1 and R2 are each independently hydrogen, C1-C10 alkyl, haloalkyl, alkoxyalkyl or C6-C12 aryl, with the proviso that the alkyl, haloalkyl and alkoxyalkyl groups may each take a straight- or branched-chain structure or a cyclic structure; and Rf1, Rf2

and Rf3 are each independently straight, branched or cyclic C1-C10 perfluoroalkyl, or alternatively Rf2 and Rf3 together with the carbon atom to which they are bonded may form C3-C8 fluorocycloalkyl. The derivs. are useful as intermediates for various organic compds. and polymers. Thus, 27.9 g 2,2-bis(4-hydroxyphenyl)hexafluoropopane was reacted with 130 g pentafluoroethylphenyliodonium trifluoromethanesulfonate in methylene chloride containing pyridine to give 18.0 g 2,2-bis(4-hydroxy-3-pentafluoroethylphenyl)hexafluoropopane.

IT 262862-13-5P 324001-97-0P 324001-98-1P

324001-99-2P

RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of bis(4-hydroxy-3-perfluoroalkylphenyl)fluoroalkane derivs.) 262862-13-5 HCAPLUS

RN 262862-13-5 HCAPLUS
CN Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 324001-97-0 HCAPLUS

CN Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 324001-98-1 HCAPLUS

CN Phenol, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

HO
$$\begin{array}{c}
\text{CF}_2-\text{CF}_2-\text{CF}_3\\
\text{CF}_3\\
\text{C-CF}_3\\
\text{CF}_2-\text{CF}_2-\text{CF}_3\\
\text{OH}
\end{array}$$

RN 324001-99-2 HCAPLUS

CN Benzene, 1,1'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[4-methoxy-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RETABLE

Referenced Author	Year	VOL	PG	Referenced Work	Referenced
(RAU)	(RPY)	(RVL)	(RPG)	(RWK)	File
=======================================	+====-	h=====+	 -	+==============	+========
Furukawa Electric Co Lt	1991			JP 345907 A	
Hoechst Ag				JP 04230228 A	HCAPLUS
Hoechst Ag				DE 4020184 A	HCAPLUS
Hoechst Ag				EP 464472 A1	HCAPLUS
Hoechst Ag				US 5118874 A	HCAPLUS
Hoechst Ag	1992	,		EP 464472 A1	HCAPLUS
Konica Corporation	2000			JP 2000105472 A	HCAPLUS
Mitsui Toatsu Chemicals	1994			JP 06116555 A	HCAPLUS
Mitsui Toatsu Chemicals	1996			JP 08179112 A	HCAPLUS
Nippon Mektron Kk				JP 07126200 A	HCAPLUS
Nippon Mektron Kk				CN 1106372 A	HCAPLUS
Nippon Mektron Kk				US 5763699 A	HCAPLUS
Nippon Mektron Kk				DE 69408085 E	
Nippon Mektron Kk	1998			EP 650949 B1	HCAPLUS
Nof Corporation	1992			JP 482855 A	ĺ
Sagami Chemical Researc	1992			JP 04283524 A	HCAPLUS
Teijin Limited	1989			JP 161706 A	

L123 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:383668 HCAPLUS

DN 133:30570

TI A process for producing perfluoroalkylaniline derivatives

IN Onishi, Masanobu; Yoshiura, Akihiko; Kohno, Eiji; Tsubata, Kenji

PA Nihon Nohyaku Co., Ltd., Japan

SO Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 2

FAN.	CNT	2														
	PAT	CENT :	NO.			KINI	DATE		API	PLICATION	NO.		D.	ATE		
													-			
ΡI	ΕP	1006	102			A2	2000	0607	EP	1999-1230	23		1	9991	119	<
	EΡ	1006	102			A3	2000	1004								
		R:	ΑT,	BE,	CH,	DE,	DK, ES,	FR,	GB, GF	R, IT, LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI, RO									
	ΑU	9959	374			A1	2000	0601	AU	1999-5937	4		1	9991	112	<
	ΑU	7317	77			B2	2001	0405								
	IN	1892	70			Α	2003	0125	IN	1999-MA11	17		1	9991	116	<
	TW	5133	93			В	2002	1211	TW	1999-8812	0170		1	9991	118	<
	ΕP	1380	568			A2	2004	0114	EP	2003-2312	0		1	9991	119	<
	EΡ	1380	568			А3	2004	0519								
		R:	CH,	DE,	FR,	GB,	IT, LI		•							
	JΡ	2001	1228	36		A2	2001	0508	. JP	1999-3387	07		1	9991	129	<
	KR	2000	03576	67		Α	2000	0626	KR	1999-5371	3		1	9991	130	<
	CN	1257	861			Α	2000	0628	CN	1999-1228	01		1	9991	130	<
	US	2002	1983	99		A1	2002	1226	US	2002-2067	69		2	0020	729	<
	US	6600	074			B2	2003	0729								
	US	2003	2041	04		A1	2003	1030	US	2003-4373	81		2	0030	514	<
	US	6717	013			B2	2004	0406								
PRAI	JP	1998	-340	354		Α	1998	1130	<							

Α	19981204	<
A	19990813	<
A3	19991119	<
B1	19991129	<
A 1	20020729	
MARPAT	133:30570	
	A A3 B1 A1	A 19990813 A3 19991119 B1 19991129

$$R^3$$
 R^4
 R^1
 R^7
 R^6
 R^6

AB Title compds. (I) [wherein R1 and R2 = independently H, (cyclo)alkyl, hydroxyalkyl, carboxyalkyl, or acyl; R3, R4, R5, R6 and R7 = independently H, halo, OH, NO2, haloalkylthio, (un) substituted aminoalkyl, Ph, benzyl, or NH2 etc.] were prepared by a process using various anilines as substrates and affording products with high position selectivity in high yield. The process uses a catalytic amount of inexpensive reaction initiating agent, an easily recoverable reaction solvent which doubles as an extraction solvent, and produces a very small amount of wastes. I are useful as raw materials for agricultural and horticultural insecticides. Thus, 2,6-dimethyl-4pentafluoroethylaniline (II) was prepared in 87% yield from 2,6-dimethylaniline and perfluoroethyl iodide in t-BuOMe/H2O with a Na2S2O4 initiator in the presence of NaHCO3 and tetrabutylammonium hydrogen sulfate. Coupling II with 6-iodo-N-isopropylphthalic acid isoimide in THF gave the insecticide III (95%). At 500 ppm III completely controlled diamondback moths and common cutworms on cabbage.

IT 226978-71-8P

CN

os GΙ

> RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (process for producing perfluoroalkylanilines from anilines and perfluoroalkyl iodides using a Na2S2O4 initiator)

RN226978-71-8 HCAPLUS

> 1,2-Benzenedicarboxamide, N1-[2,6-dimethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-3-iodo-N2-(1-methylethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH}_2 \\ \text{CF}_2 - \text{CF}_3 \end{array}$$

```
226979-96-0P, 2-Methyl-4-pentafluoroethylaniline
238098-26-5P, 2-Methyl-4-heptafluoroisopropylaniline
238098-28-7P; 2-Methyl-4-(nonafluorobutyl)aniline
257868-17-0P, 2,6-Dimethyl-4-perfluorooctylaniline
273735-33-4P, 3-Methyl-4-heptafluoroisopropylaniline
273735-34-5P, 2-Ethyl-4-heptafluoroisopropylaniline
273735-35-6P, 2-Isopropyl-4-heptafluoroisopropylaniline
273735-41-4P, 4-Heptafluoroisopropyl-2,3-dimethylaniline
273735-42-5P, 4-Heptafluoroisopropyl-2,5-dimethylaniline
273735-43-6P, 4-Heptafluoroisopropyl-2,6-dimethylaniline
273735-44-7P, 4-Heptafluoroisopropyl-2,6-diethylaniline
273735-45-8P, 4-Heptafluoroisopropyl-2,6-diisopropylaniline
273735-46-9P, 5-Fluoro-4-heptafluoroisopropyl-2-methylaniline
273735-47-0P, 5-Chloro-4-heptafluoroisopropyl-2-methylaniline
273735-48-1P, 4-Heptafluoroisopropyl-N,2-dimethylaniline
273735-52-7P, 4-tert-Butyl-2-heptafluoroisopropylaniline
273735-53-8P, 2-Heptafluoroisopropyl-4-methylaniline
273735-55-0P, 2-Methyl-4-perfluorooctylaniline
273735-57-2P, 2,6-Diethyl-4-pentafluoroethylaniline
273735-59-4P, 4-tert-Butyl-2-pentafluoroethylaniline
273735-60-7P, 2,6-Dimethyl-4-heptafluoropropylaniline
273735-62-9P, 4-Heptafluoroisopropyl-2-hydroxy-5-methylaniline
273735-68-5P, 2-Heptafluoroisopropyl-4-isopropylaniline
273735-70-9P, 2-Heptafluoroisopropyl-5-(1-hydroxyethyl)aniline
273735-72-1P, 4-Heptafluoroisopropyl-3-hydroxymethylaniline
273735-73-2P, 4-Heptafluoroisopropyl-2-(1-hydroxyethyl)aniline
273735-74-3P, 4-Heptafluoroisopropyl-2-(4-methylpentan-2-
yl)aniline 273735-75-4P, 3,5-Dimethyl-2-
heptafluoroisopropylaniline 273735-79-8P, N-Acetyl-4-
heptafluoroisopropyl-2-methylaniline 273735-80-1P,
4-Heptafluoroisopropyl-N-methoxycarbonyl-2-methylaniline
273735-81-2P, N-tert-Butoxycarbonyl-2-fluoromethyl-4-
heptafluoroisopropylaniline 273735-82-3P 273735-83-4P,
N-tert-Butoxycarbonyl-4-heptafluoroisopropyl-2-(hydroxymethyl) aniline
273735-84-5P, N-tert-Butoxycarbonyl-2-chloromethyl-4-
heptafluoroisopropylaniline 273735-85-6P 273735-86-7P,
2-(Hydroxymethyl)-4-heptafluoroisopropyl-N-methoxycarbonylaniline
273735-92-5P, 4-Heptafluoroisopropyl-5-(hydroxymethyl)-2-
methylaniline 273735-93-6P, 4-Acetyl-2-
heptafluoroisopropylaniline 273735-94-7P, 2-Ethyl-4-
heptafluoroisopropyl-6-methylaniline 273735-95-8P,
2,6-Dimethyl-4-nonafluorobutylaniline 273735-96-9P,
2,6-Dimethyl-4-perfluorohexylaniline 273735-97-0P,
2,6-Diethyl-4-nonafluorobutylaniline 273735-98-1P,
2,6-Diethyl-4-perfluorohexylaniline 273735-99-2P,
```

2-(Hydroxymethyl)-4-perfluorohexylaniline

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process for producing perfluoroalkylanilines from anilines and perfluoroalkyl iodides using a Na2S2O4 initiator)

RN 226979-96-0 HCAPLUS

CN Benzenamine, 2-methyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

$$H_2N$$
 Me
 CF_2-CF_3

RN 238098-26-5 HCAPLUS

CN Benzenamine, 2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

RN 238098-28-7 HCAPLUS

CN Benzenamine, 2-methyl-4-(nonafluorobutyl)- (9CI) (CA INDEX NAME)

RN 257868-17-0 HCAPLUS

CN Benzenamine, 4-(heptadecafluorooctyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)

Me (CF₂)₇-CF₃

$$H_2N$$
Me

RN 273735-33-4 HCAPLUS

CN Benzenamine, 3-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

RN 273735-34-5 HCAPLUS

CN Benzenamine, 2-ethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

RN 273735-35-6 HCAPLUS

CN Benzenamine, 2-(1-methylethyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 273735-41-4 HCAPLUS

CN Benzenamine, 2,3-dimethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & F \\ \hline \\ \text{C-CF}_3 \\ \\ \text{H}_2 \text{N} \end{array}$$

RN 273735-42-5 HCAPLUS

CN Benzenamine, 2,5-dimethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CF3} \\ | \\ \text{C-CF3} \\ | \\ \text{H}_2\text{N} \end{array}$$

RN 273735-43-6 HCAPLUS

CN Benzenamine, 2,6-dimethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & & F \\ | & \\ \text{C-CF}_3 \\ \\ \text{H}_2\text{N} & \\ \text{Me} & \end{array}$$

RN 273735-44-7 HCAPLUS

CN Benzenamine, 2,6-diethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

RN 273735-45-8 HCAPLUS

CN Benzenamine, 2,6-bis(1-methylethyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 273735-46-9 HCAPLUS

CN Benzenamine, 5-fluoro-2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CF3} \\ | \\ \text{C-CF3} \\ \\ \text{F} \\ \\ \text{F} \end{array}$$

RN 273735-47-0 HCAPLUS
CN Benzenamine, 5-chloro-2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & CF_3 \\ & C-CF_3 \\ & F \\ & C1 \end{array}$$

RN 273735-48-1 HCAPLUS
CN Benzenamine, N,2-dimethyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl](9CI) (CA INDEX NAME)

RN 273735-52-7 HCAPLUS
CN Benzenamine, 4-(1,1-dimethylethyl)-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 273735-53-8 HCAPLUS
CN Benzenamine, 4-methyl-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl](9CI) (CA INDEX NAME)

RN 273735-55-0 HCAPLUS

CN Benzenamine, 4-(heptadecafluorooctyl)-2-methyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 Me
 $(CF_2)_7-CF_3$

RN 273735-57-2 HCAPLUS

CN Benzenamine, 2,6-diethyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 273735-59-4 HCAPLUS

CN Benzenamine, 4-(1,1-dimethylethyl)-2-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 273735-60-7 HCAPLUS

CN Benzenamine, 4-(heptafluoropropyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)

RN 273735-62-9 HCAPLUS

CN Phenol, 2-amino-4-methyl-5-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

RN 273735-68-5 HCAPLUS

CN Benzenamine, 4-(1-methylethyl)-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 273735-70-9 HCAPLUS

Benzenemethanol, $3-amino-\alpha-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)$

RN 273735-74-3 HCAPLUS

CN Benzenamine, 2-(1,3-dimethylbutyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 273735-75-4 HCAPLUS

CN Benzenamine, 3,5-dimethyl-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

RN 273735-79-8 HCAPLUS

CN Acetamide, N-[2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 273735-80-1 HCAPLUS

CN Carbamic acid, [2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 273735-81-2 HCAPLUS

CN Carbamic acid, [2-(fluoromethyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273735-82-3 HCAPLUS

CN Carbamic acid, [2-[(dimethylamino)methyl]-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273735-83-4 HCAPLUS

CN Carbamic acid, [2-(hydroxymethyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273735-84-5 HCAPLUS

CN Carbamic acid, [2-(chloromethyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 273735-85-6 HCAPLUS

CN Carbamic acid, [2-[(dimethylamino)methyl]-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 273735-86-7 HCAPLUS

CN Carbamic acid, [2-(hydroxymethyl)-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 273735-92-5 HCAPLUS

CN Benzenemethanol, 5-amino-4-methyl-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

RN 273735-93-6 HCAPLUS

CN Ethanone, 1-[4-amino-3-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 273735-94-7 HCAPLUS

CN Benzenamine, 2-ethyl-6-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & F \\ \hline \\ C - CF_3 \\ \hline \\ CF_3 \\ \hline \\ Me \end{array}$$

RN 273735-95-8 HCAPLUS

CN Benzenamine, 2,6-dimethyl-4-(nonafluorobutyl)- (9CI) (CA INDEX NAME)

RN 273735-96-9 HCAPLUS

CN Benzenamine, 2,6-dimethyl-4-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

Me (CF₂)₅-CF₃

$$H_2N$$
Me

RN 273735-97-0 HCAPLUS

CN Benzenamine, 2,6-diethyl-4-(nonafluorobutyl)- (9CI) (CA INDEX NAME)

RN 273735-98-1 HCAPLUS

CN Benzenamine, 2,6-diethyl-4-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

RN 273735-99-2 HCAPLUS

CN Benzenemethanol, 2-amino-5-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

IT 273736-01-9, 2-Methyl-6-heptafluoroisopropylaniline

273736-03-1, 2-Methyl-6-nonafluorobutylaniline 273736-04-2

, 2-Methyl-6-perfluorooctylaniline

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for producing perfluoroalkylanilines from anilines and

perfluoroalkyl iodides using a Na2S2O4 initiator)

RN 273736-01-9 HCAPLUS

CN Benzenamine, 2-methyl-6-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{NH}_2 & F \\ \hline & C - CF_3 \\ \hline & CF_3 \end{array}$$

RN 273736-03-1 HCAPLUS

CN Benzenamine, 2-methyl-6-(nonafluorobutyl)- (9CI) (CA INDEX NAME)

RN 273736-04-2 HCAPLUS

CN Benzenamine, 2-(heptadecafluorooctyl)-6-methyl- (9CI) (CA INDEX NAME)

273735-56-1P, 2,6-Dimethyl-4-pentafluoroethylaniline
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (target intermediate for insecticide production; process for producing perfluoroalkylanilines from anilines and perfluoroalkyl iodides using a Na2S2O4 initiator)

RN 273735-56-1 HCAPLUS

CN Benzenamine, 2,6-dimethyl-4-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

L123 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:87742 HCAPLUS

DN 124:232039

TI Preparation of (perfluoroalkyl)phenols from halophenols

IN Iwahara, Masahiro

PA Idemitsu Petrochemical Co, Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

F	PATENT NO.	KIND DATE		APPLICATION NO.	DATE			
-								
PI J	JP 07304702	A2	19951121	JP 1994-94473	19940506 <			
PRAI J	JP 1994-94473		19940506	<				

OS CASREACT 124:232039

AB (Perfluoroalkyl)phenols, useful as terminating agents for polycarbonate manufacture and materials and components for liquid-crystal display devices, surfactants, etc., are prepared by treatment of halophenols with C1-20 perfluoroalkyl iodides in the presence of metal Cu catalyst. A mixture of C10F21I, p-IC6H4OH, Cu powder, and DMSO was heated at 120° for 15 h to give 72% p-C10F21C6H4OH.

IT 174611-78-0P 174611-79-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of (perfluoroalkyl) phenols from halophenols and perfluoroalkyl iodides using metal Cu catalyst)

RN 174611-78-0 HCAPLUS

CN Phenol, 3,4-bis(tridecafluorohexyl) - (9CI) (CA INDEX NAME)

RN 174611-79-1 HCAPLUS

CN Phenol, 3,4-bis(heneicosafluorodecyl) - (9CI) (CA INDEX NAME)

L123 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

N 1994:244325 HCAPLUS

DN 120:244325

TI Polyfluoroalkylation of aromatic compounds and polymers

IN May, Donald Douglas

PA du Pont de Nemours, E. I., and Co., USA

SO PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

11111	OIVI D			
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
PI	WO 9316969	A1 19930902	WO 1993-US1459	19930224 <
	W: AU, CA, FI,	JP, KR, NO		
	RW: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IE, IT, LU, MC,	NL, PT, SE
	AU 9337245	A1 19930913	AU 1993-37245	19930224 <
	EP 628019	A1 19941214	EP 1993-906064	19930224 <
	EP 628019	B1 19970423		
	R: DE, FR, GB,	NL		
	JP 07504414 `	T2 19950518	JP 1993-514955	19930224 <
PRAI	US 1992-843749	A 19920228	<	
	US 1992-843885	A 19920228	<	
	WO 1993-US1459	A 19930224	<	
os	CASREACT 120:244325			

AB Polyfluorinated aromatic compds. or polymers are prepared by reaction of aromatic

compds. or aromatic polymers (which are subject to electrophilic attack) with a C1-20 polyfluoroalkyl iodide in the presence of an aqueous alkali or alkaline earth hydroxide or (bi)carbonate and a catalyst containing ≥1 of Rh, Pd, Pt, Ru, Cu, Ni, Re, or Co. For example, reaction of benzene with CF3(CF2)3I (I) in 50% aq K2CO3 in the presence of a silica-supported catalyst containing 2% Pd and 0.1% Pt at 170° for 30 h gave complete conversion of I, and produced (perfluorobutyl)benzene and mixed isomers of di(perfluorobutyl)benzene in yields of 93% and 5%, resp. The identical reaction without H2O gave yields of only 55% and 1%, with 43% unreacted I. Other examples of perfluoroalkylation using I included naphthalene, anthracene, PhCN (with concomitant hydrolysis), PhMe, PhOH, PhAc, PhOMe, and p-ClC6H4NH2. Mixed C4-10 perfluoroalkyl (telomer) iodides were used

with benzene, styrene-maleic acid copolymer, polystyrene, and polystyrene sulfonate Na salt.

IT 152330-63-7P 152330-64-8P 152330-65-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of perfluoroalkylated aroms. and aromatic polymers)

RN 152330-63-7 . HCAPLUS

CN Ethanone, 1-[2-(nonafluorobutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 152330-64-8 HCAPLUS

CN Ethanone, 1-[3-(nonafluorobutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 152330-65-9 HCAPLUS

CN Ethanone, 1-[4-(nonafluorobutyl)phenyl]- (9CI) (CA INDEX NAME)

L123 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:216928 HCAPLUS

DN 120:216928

TI Process and catalysts for the perfluoroalkylation of aromatic hydrocarbons

IN May, Donald D.

PA du Pont de Nemours, E. I., and Co., USA

SO U.S., 6 pp. Cont.-in-part of U.S. Ser. No. 843,749, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
				
PI US 5276194	Α	19940104	US 1993-59184	19930507 <
PRAI US 1992-843749	B2	19920228	<	

OS CASREACT 120:216928

AB Aromatic hydrocarbons are effectively perfluoroalkylated by reacting a perfluoroalkyl iodide with the aromatic hydrocarbon in the presence of a platinum group metal catalyst and an aqueous inorg. base selected from alkaline metal and alkaline earth metal hydroxides, carbonates, and bicarbonates. Thus, C6H6, ICF2CF2CF3, 50% aqueous K2CO3 solution, and a catalyst consisting

of 2% Pd and 0.1% Pt on a silica support was heated with stirring for 30 h at 170°, producing a 93% yield of PhCF2CF2CF3 and a 5% yield of mixed dye (perfluorobutyl)benzene isomers.

RN 152330-63-7 HCAPLUS

CN Ethanone, 1-[2-(nonafluorobutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 152330-64-8 HCAPLUS

CN Ethanone, 1-[3-(nonafluorobutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 152330-65-9 HCAPLUS

CN Ethanone, 1-[4-(nonafluorobutyl)phenyl]- (9CI) (CA INDEX NAME)

RN 153910-94-2 HCAPLUS

CN Benzene, 1,2-bis(nonafluorobutyl) - (9CI) (CA INDEX NAME)

RN 153910-95-3 HCAPLUS

CN Benzene, 1,3-bis(nonafluorobutyl) - (9CI) (CA INDEX NAME)

RN 153910-96-4 HCAPLUS

CN Benzene, 1,4-bis(nonafluorobutyl) - (9CI) (CA INDEX NAME)

```
F_3C-(CF_2)_3
                    (CF_2)_3 - CF_3
L123 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
     1992:151298 HCAPLUS
ΑN
DN
     116:151298
TI
     Preparation of perfluoroalkylbenzenes or -naphthalenes
     Kamigata, Nobumasa; Yoshida, Masato; Sawada, Hideo; Nakayama, Masaharu
TN
     Nippon Oil and Fats Co., Ltd., Japan
PΑ
     Jpn. Kokai Tokkyo Koho, 6 pp.
SO
     CODEN: JKXXAF
DT
    Patent
LA
    Japanese
FAN.CNT 1
     PATENT NO.
                       KIND
                                          APPLICATION NO.
                               DATE
                                                                DATE
                               -----
                       ----
                                           -----
                                                                  _____
     JP 03240739
                        A2
                                          JP 1990-32419
PΙ
                               19911028
                                                                19900215 <--
                              19900215 <--
PRAI JP 1990-32419
     CASREACT 116:151298; MARPAT 116:151298
os
AΒ
     Aromatic compds. are treated with F(CF2) nSO2Cl (n = 1-20) in the presence of
     metal catalysts to introduce fluoroalkyl groups into benzene or
     naphthalene rings of the aromatic compds. 1,4-Dimethoxybenzene was treated
     with perfluorohexanesulfonyl chloride and (Ph3P)3RuCl2 at 120° for
     24 h to give 81% 1,4-dimethoxy-2-perfluorohexylbenzene.
IT
     123524-58-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, by perfluoroalkylation with perfluoroalkanesulfonyl
        chloride)
     123524-58-3 HCAPLUS
RN
CN
     Benzene, 1,4-dimethyl-2-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)
     (CF_2)_5 - CF_3
           Me
Me
LA23 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ΔN
     1992:20793 HCAPLUS
     116:20793
DN
ΤI
     Preparation of perfluoroalkyl group containing compounds
IN
     Fuchigami, Takamasa; Urata, Hisao
     Sagami Chemical Research Center, Japan
PA
     Jpn. Kokai Tokkyo Koho, 12 pp.
SO
     CODEN: JKXXAF
DТ
    Patent
LA
    Japanese
FAN.CNT 1
                       KIND
    PATENT NO.
                               DATE
                                          APPLICATION NO.
                                                                 DATE
```

19910925

19891102 <--

JP 1990-59885

19900313 <--

CASREACT 116:20793; MARPAT 116:20793

JP 03218325

PRAI JP 1989-284746

PΙ

A2 A1 AB Title compds. CnF2n+1R [R = (un)substituted aryl, aralkyl, alkenyl; n = 1-10] were prepared by reaction of RX (X = Br, iodo) with CnF2n+1SiR1R2R3 (R1, R2, R3 = alkyl) in the presence of Cu salts and fluoride ion sources. Thus, stirring 4-O2NC6H4I with CF3SiEt3, CuI, and KF in DMF under Ar at 80° for 24 h gave 86% 4-O2NC6H4CF3.

IT 133512-60-4P

RN 133512-60-4 HCAPLUS

CN Benzoic acid, 4-(pentafluoroethyl)-, ethyl ester (9CI) (CA INDEX NAME)

L123 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:631878 HCAPLUS

DN 115:231878

TI Preparation of fluoroalkyl aromatic nitrogen compounds

IN Mitani, Motohiro; Sawada, Hideo; Nakayama, Masaharu

PA Nippon Oil and Fats Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

L-MIN.	-1/1 T						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	JP 03109362	A2	19910509	JP 1989-286026	19891104 <		
	JP 2775913	B2	19980716				
PRAI	JP 1989-139160	A1	19890602 <	<			
os	CASREACT 115:231878;	MARPAI	r 115:231878	3			
GI							

$$R^{1}NH$$
 $(CF_{2})_{n}X$
 I
 $R^{3}NH$
 $(CF_{2})_{2}CF_{3}$
 $NHAC$
 $NHAC$
 III

AB Title compds., e.g. I (R1, R2 = H, acyl, fluoroacyl; X = H, Cl, F; n = 1-10) were prepared by fluoroalkylation of compds. II (R3, R4 = acyl, fluoroacyl) with X(CF2)nCO2O2C(CF)nX. E.g., treating N,N'-diacetyl-p-phenylenediamine with bis(heptafluorobutyryl) peroxide in 1,1,2-trichlorotrifluoroethane at 40° for 5 h gave 56%

CN Acetamide, N-[4-[4-(acetylamino)-3,5-dimethylphenoxy]-3-(heptafluoropropyl)-2,6-dimethylphenyl]- (9CI) (CA INDEX NAME)

RN 135977-30-9 HCAPLUS
CN Acetamide, N,N'-[oxybis[3-(heptafluoropropyl)-2,6-dimethyl-4,1phenylene]]bis- (9CI) (CA INDEX NAME)

$$F_3C-CF_2-CF_2$$

Me

NHAC

Me

 $CF_2-CF_2-CF_3$

RN 135977-31-0 HCAPLUS
CN Acetamide, N-[4-[1-[4-(acetylamino)-3-(heptafluoropropyl)phenyl]-2,2,2-trifluoro-1-(trifluoromethyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 135977-32-1 HCAPLUS

CN Acetamide, N,N'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-(heptafluoropropyl)-4,1-phenylene]]bis-(9CI) (CA INDEX NAME)

$$CF_3$$
 CF_3
 CF_3
 CF_3
 CF_3
 CF_3
 CF_2
 CF_2
 CF_2
 CF_2
 CF_3

RN 135977-35-4 HCAPLUS

CN Acetamide, N-[4-[4-(acetylamino)-3,5-dimethylphenoxy]-2,6-dimethyl-3-(tridecafluorohexyl)phenyl]- (9CI) (CA INDEX NAME)

RN 135977-36-5 HCAPLUS

CN Acetamide, N,N'-[oxybis[2,6-dimethyl-3-(tridecafluorohexyl)-4,1-phenylene]]bis- (9CI) (CA INDEX NAME)

Me
$$(CF_2)_5 - CF_3$$
Me $(CF_2)_5$
Me $(CF_2)_5$
Me $(CF_2)_5$
Me $(CF_2)_5$

RN 135977-37-6 HCAPLUS

CN Acetamide, N-[4-[1-[4-(acetylamino)phenyl]-2,2,2-trifluoro-1-(trifluoromethyl)ethyl]-3-(tridecafluorohexyl)phenyl]- (9CI) (CA INDEX NAME)

RN 135977-38-7 HCAPLUS

CN Acetamide, N,N'-[[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-(tridecafluorohexyl)-4,1-phenylene]]bis- (9CI) (CA INDEX NAME)

IT 135977-41-2P 135977-42-3P 135977-43-4P 135977-44-5P 135977-47-8P 135977-48-9P

135977-49-0P 136507-93-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 135977-41-2 HCAPLUS

CN Benzenamine, 4-(4-amino-3,5-dimethylphenoxy)-3-(heptafluoropropyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{NH}_2 \\ \\ \text{Me} \\ & \text{CF}_2 - \text{CF}_2 - \text{CF}_3 \\ \\ & \text{Me} \end{array}$$

RN 135977-42-3 HCAPLUS

CN Benzenamine, 4,4'-oxybis[3-(heptafluoropropyl)-2,6-dimethyl- (9CI) (CA INDEX NAME)

RN 135977-43-4 HCAPLUS

CN Benzenamine, 4-[1-(4-aminophenyl)-2,2,2-trifluoro-1-(trifluoromethyl)ethyl]-2-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

$$CF_3$$
 CF_3
 CF_3
 CF_2
 CF_2
 CF_2
 CF_3

RN 135977-44-5 HCAPLUS

CN Benzenamine, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-

(heptafluoropropyl) - (9CI) (CA INDEX NAME)

$$CF_3$$
 CF_3
 CF_3
 CF_3
 CF_3
 CF_3
 CF_3
 CF_3
 CF_3
 CF_2
 CF_3
 CF_3

RN 135977-47-8 HCAPLUS

CN Benzenamine, 4-(4-amino-3,5-dimethylphenoxy)-2,6-dimethyl-3-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CF}_2\text{)}_5\text{--}\text{CF}_3\\ \text{Me} & \text{Me} & \text{NH}_2\\ \text{Me} & \text{Me} & \text{Me} \end{array}$$

RN 135977-48-9 HCAPLUS

CN Benzenamine, 4,4'-oxybis[2,6-dimethyl-3-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CF}_2) \ 5 - \text{CF}_3 \\ \text{Me} & \text{O} \\ \text{H}_2\text{N} & \text{CF}_2) \ 5 & \text{Me} \\ \text{CF}_3 & \text{Me} \end{array}$$

RN 135977-49-0 HCAPLUS

CN Benzenamine, 4-[1-(4-aminophenyl)-2,2,2-trifluoro-1-(trifluoromethyl)ethyl]-3-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

RN 136507-93-2 HCAPLUS

CN Benzenamine, 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[2-(tridecafluorohexyl)- (9CI) (CA INDEX NAME)

```
CF<sub>3</sub>
               CF<sub>3</sub>
H<sub>2</sub>N
                             NH<sub>2</sub>
       (CF<sub>2</sub>)<sub>5</sub>-CF<sub>3</sub>
                     (CF_2)_5 - CF_3
L123 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
AN
      1991:607657 HCAPLUS
DN
      115:207657
     Manufacture of fluorine-containing benzaldehyde derivatives
ΤI
IN
     Mitani, Motohiro; Sawada, Hideo; Nakayama, Masaharu
     Nippon Oil and Fats Co., Ltd., Japan
PΑ
     Jpn. Kokai Tokkyo Koho, 5 pp.
SO
     CODEN: JKXXAF
DT
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                             KIND
                                     DATE
                                                    APPLICATION NO.
                                                                               DATE
PI
     JP 03123751
                              A2
                                      19910527
                                                    JP 1989-260200
                                                                               19891006 <--
PRAI JP 1989-260200
                                      19891006 <--
os
     CASREACT 115:207657; MARPAT 115:207657
GΙ
```

$$(R)_n$$
 $(CF_2)_mX$ $(R)_n$ $(R)_n$

AB Title derivs. I (R = halo, C1-4 alkyl, C1-4 alkoxy, C1-4 alkoxycarbonyl, CO2H, OH, C1-4 alkanesulfonyl; X = F, Cl, H; m = 1-10; n = 0-4; m = 10when n = 0 or 1 and R = halo) are manufactured by the reaction of benzaldehydes II with X(F2C)mCOO2CO(CF2)mX. Thus, treating benzaldehyde with bis (heptafluorobutyryl) peroxide in 1,1,2-trichlorotrifluoroethane at 40° under N gave 90% 3-heptafluoropropylbenzaldehyde. IT 131608-36-1P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN131608-36-1 HCAPLUS Benzene, 1-ethenyl-3-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

CN

IT 136850-59-4P, 3-Heptafluoropropylbenzaldehyde 136850-60-7P , 3-Heptafluoropropyl-4-methoxybenzaldehyde 136850-61-8P, 3-Heptafluoropropyl-4-hydroxybenzaldehyde 136850-62-9P, 3-Heptafluoropropyl-4-methylbenzaldehyde

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by perfluoroalkylation with bis(heptafluorobutyryl) peroxide)

RN 136850-59-4 HCAPLUS

CN Benzaldehyde, 3-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

RN 136850-60-7 HCAPLUS

CN Benzaldehyde, 3-(heptafluoropropyl)-4-methoxy- (9CI) (CA INDEX NAME)

RN 136850-61-8 HCAPLUS

CN Benzaldehyde, 3-(heptafluoropropyl)-4-hydroxy- (9CI) (CA INDEX NAME)

RN 136850-62-9 HCAPLUS

CN Benzaldehyde, 3-(heptafluoropropyl)-4-methyl- (9CI) (CA INDEX NAME)

L123 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:121712 HCAPLUS

DN 114:121712

TI Preparation of perfluoroalkylnitrobenzenes as intermediates for drugs and agrochemicals

IN Powell, Richard Llewellyn; Heaton, Charles Alan

PA Imperial Chemical Industries PLC, UK

SO Eur. Pat. Appl., 5 pp.

CODEN: EPXXDW

DT Patent

LA English FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	EP 395342	A2	19901031	EP 1990-304360	19900424 <
	EP 395342	A3	19920129		

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE

JP 02295945 A2 19901206 JP 1990-108985 19900426 <--US 5113013 Α 19920512 US 1990-515509 19900426 <--

PRAI GB 1989-9574 Α 19890426 <--

MARPAT 114:121712

AB Fluorine-containing organic compds. were prepared by reacting a sulfonyl halide of

the formula: RfSO2X (Rf = fluorinated organic radical and X = halo) with a reactive organic halide in the presence of a metal known to complex with fluorinated organic radicals. Treatment of 2-nitrobromobenzene with CF3SO2Cl in DMF containing copper at 140° for 1 h gave 2nitrotrifluoromethylbenzene.

132502-10-4P 132502-12-6P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN132502-10-4 HCAPLUS

Benzene, 1,4-dinitro-2-(tridecafluorohexyl)-5-(trifluoromethyl)- (9CI) CN (CA INDEX NAME)

$$CF_2$$
 CF_3 CF_3 CF_3 CF_3

RN132502-12-6 HCAPLUS

Benzene, 2-(heptadecafluorooctyl)-1,3-dinitro-5-(trifluoromethyl)- (9CI) CN (CA INDEX NAME)

$$rac{NO_2}{(CF_2)_7 - CF_3}$$
 $rac{NO_2}{NO_2}$

LI23 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:61676 HCAPLUS

DN

TI Fluoroalkyl-containing aromatic compounds and their preparation

Sawada, Hideo; Mitani, Motohiro; Nakayama, Masaharu TN

PA Nippon Oils & Fats Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DT Patent

Japanese LA

FAN.CNT 1

PATENT NO. KIND APPLICATION NO. DATE DATE

PI JP 02200646 PRAI JP 1989-19871 OS MARPAT 114:61676 GI A2 19900808 JP 1989-19871 19890131 <-- 19890131 <--

Gı

$$CH = CH_2$$
 $CHR^2CH_2R^3$
 $(R^4)_m$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$
 $(CF_2)_nF$

AB The title compds. I (R1 = H, C1-4 alkyl, alkoxy; m = 0, 1; n = 1-10) and II (R2 = C1, Br, F, OH, Me3SiO, (Me3C)Me2SiO, AcO, MeSO3; R3 = H, C1, Br,F; R4 = H, C1-4 alkyl, alkoxy; m, n = same as I) are prepared II are prepared by treatment of I with acids or alkalies. Bis(perfluorobutyryl) peroxide in CF2ClCFCl2 was treated with (2-chloroethyl)benzene at 40° for 5 h to give 56% 1-(2-chloroethyl)-4-perfluoropropylbenzene, which was refluxed with KOH in MeOH for 5 h to afford 93% p-perfluoropropylstyrene. IT 131608-23-6P 131608-24-7P 131608-25-8P 131608-26-9P 131608-27-0P 131608-28-1P 131608-29-2P 131608-30-5P 131608-31-6P 131608-32-7P 131608-33-8P 131608-34-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and elimination reaction of) 131608-23-6 HCAPLUS Benzene, 1-(2-chloroethyl)-4-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

RN 131608-26-9 HCAPLUS

CN Benzene, 1-(2-chloroethyl)-4-(pentadecafluoroheptyl)- (9CI) (CA INDEX NAME)

RN 131608-31-6 HCAPLUS CN Benzenemethanol, 2-(heptafluoropropyl)- α -methyl- (9CI) (CA INDEX

NAME)

Me-CH
$$CF_2-CF_2-CF_3$$

RN 131608-34-9 HCAPLUS CN Benzene, 1-(1-chloroethyl)-2-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

RN 131608-35-0 HCAPLUS

CN Benzene, 1-ethenyl-4-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

$$CF_2-CF_2-CF_3$$

RN 131608-36-1 HCAPLUS

CN Benzene, 1-ethenyl-3-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

RN 131608-37-2 HCAPLUS

CN Benzene, 1-ethenyl-2-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

RN 131608-38-3 HCAPLUS

CN Benzene, 1-ethenyl-3-(pentadecafluoroheptyl)- (9CI) (CA INDEX NAME)

RN 131608-39-4 HCAPLUS

CN Benzene, 1-ethenyl-2-(pentadecafluoroheptyl)- (9CI) (CA INDEX NAME)

L123 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:440144 HCAPLUS

DN 113:40144

- TI Preparation of perfluoroalkylphenols and -naphthols as drug and agrochemical intermediates
- IN Sawada, Hideo; Mitani, Motohiro; Nakayama, Masaharu; Akusawa, Kazuko
- PA Nippon Oils & Fats Co., Ltd., Japan
- SO Jpn. Kokai Tokkyo Koho, 10 pp. CODEN: JKXXAF

DT Patent LA Japanese FAN.CNT 1

GΙ

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
			-				
ΡI	JP 02059535	A2	19900228	JP 1988-210662	19880826 <		
PRAI	JP 1988-210662		19880826	<			
os	MARPAT 113:40144						

$$(X^1)_a$$

$$[(CF_2)_nX^2]_m$$
 $(R^1)_b$

$$\begin{bmatrix} X^2 (CF_2)_n \end{bmatrix}_z \qquad (X^1)_a$$

$$(R^1)_b \qquad (CF_2)_n X^2 \qquad II$$

AB The title compds. I [X1 = OH, CO2H, C1-4 alkoxycarbonyl; R1 = halo, C1-4 alkyl, NO2, cyano, etc.; X2 = F, Cl, H; a = 1-3; b = 0-2; n = 1-10; m = 1, 2] and II (z = 0-1; other variables = as given above) were prepared by perfluoroalkylation of aromatic compds. with X2(CF2)nC(:0)OOC(:0)(CF2)nX2. A solution of bis(heptafluorobutyryl)peroxide in 1,1,2-trichlorotirfluoroethane was treated with PhOH at 40° for 5 h to give 93% (heptafluoropropyl)phenol.

IT 128133-78-8P 128133-79-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as drug and agrochem. intermediate)

Ι

RN 128133-78-8 HCAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(heptafluoropropyl)- (9CI) (CA INDEX NAME)

RN 128133-79-9 HCAPLUS

CN 1,4-Benzenedicarboxylic acid, 2-(heptafluoropropyl)-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} R1 & \\ \hline & R^2 & I \end{array}$$

Ethanone, 1-[2-(heptadecafluorooctyl)phenyl]- (9CI) (CA INDEX NAME)

CN

RN 83766-57-8 HCAPLUS CN Ethanone, 1-[4-(heptadecafluorooctyl)phenyl]- (9CI) (CA INDEX NAME)

RN 83766-58-9 HCAPLUS

CN Benzoic acid, 2-(heptadecafluorooctyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 83766-59-0 HCAPLUS

CN Benzoic acid, 4-(heptadecafluorooctyl)-, ethyl ester (9CI) (CA INDEX NAME)

L123 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1982:438657 HCAPLUS

DN 97:38657

TI Perfluoroalkyl-substituted benzene derivatives

PA Sagami Chemical Research Center, Japan

SO Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		,		
PI JP 57018638	A2	19820130	JP 1980-91790	19800707 <
PRAI JP 1980-91790	Α	19800707	<	

AB Ten perfluoroalkyl-substituted benzene derivs. RC6H3R1R2 [R, R1 = H, halo, alkyl, alkoxy, (un)substituted NH2; at least one of R and R1 is (un)substituted NH2 or alkyl; R2 = perfluoroalkyl] were prepared by perfluoroalkylation of RC6H4R1 with R2I in the presence of reducing agents under UV irradiation Thus, a mixture of 1 g n-C8F17I and 40 mL 5% aqueous NaHSO3 in

PhMe was stirred 10 h under a high pressure Hg lamp to give 290 mg o-, m-, and p-C8F17C6H4Me.

IT 82396-49-4P 82396-50-7P 82396-51-8P

82396-52-9P 82396-53-0P 82396-55-2P

RN 82396-49-4 HCAPLUS

CN Benzene, 1-(heptadecafluorooctyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 82396-50-7 HCAPLUS

CN Benzene, 1-(heptadecafluorooctyl)-3-methyl- (9CI) (CA INDEX NAME)

RN 82396-51-8 HCAPLUS

CN Benzene, 1-(heptadecafluorooctyl)-4-methyl- (9CI) (CA INDEX NAME)

RN 82396-52-9 HCAPLUS

CN' Benzene, 2-(heptadecafluorooctyl)-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 82396-53-0 HCAPLUS

CN Benzene, 4-bromo-2-(heptafluoropropyl)-1-methyl- (9CI) (CA INDEX NAME)

RN 82396-55-2 HCAPLUS

CN Benzene, 1-bromo-2-(heptafluoropropyl)-4-methyl- (9CI) (CA INDEX NAME)

```
Me
       CF2-CF2-CF3
123 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN AN 1969:57375 HCAPLUS
DN
     70:57375
ΤI
     Fluoroalkyl aromatics
TN
     McLoughlin, Victor C. R.; Thrower, John
     Minister of Technology
PA
SO
     U.S., 5 pp.
     CODEN: USXXAM
DT
     Patent
LA
     English
FAN.CNT 2
     PATENT NO.
                        KIND
                                DATE
                                           APPLICATION NO.
                                                                    DATE
                         ----
PI
     US 3408411
                          Α
                                19681029
                                          US 1967-654980
                                                                    19670721 <--
     GB 1156912
                         Α
                                19690702
                                          GB 1965-21636
                                                                    19650521 <--
PRAI GB 1965-21636
                         Α
                                19650521 <--
     A series of title compds. of the type ArR (I) or Ar2R (II) were prepared by
     the interaction of an aromatic iodide, a perfluoroalkyl halide, and Cu
     bronze (III). Thus a mixture of 15.5 g. PhI and 10 g. III in 45 ml. Me2NCHO
     was stirred at reflux as 10 g. n-C3F7I was added beneath the surface over
     1 hr., and the mixture refluxed 90 min. and worked up to give 39% I (Ar =
     Ph, R = n-C3F7), b. 130.2°. Similarly were prepared the following
     compds. (compound type, Ar, R, m.p., b.p./mm., and % yield given): I, Ph,
     EtO2C(CF2)3, -, 130-2°/20, 45; I, Ph, n-C7H15, -, -, >30; I,
     o-O2NC6H4, n-C7F15, -, 120-5°/35, 15-20; I, Ph, F3CCH2, -,
     115-20°, 10-15; II, Ph, (CF2)3, -, 133°/5, 60; II,
     3-pyridyl, (CF2)3, 63°, -, 53; II, m-MeC6H4, (CF2)3, -,
     160-2°/18, 65; II, m-MeOC6H4, (CF2)3, -, 146-50°/0.2, 55;
     II, m-AcOC6H4, (CF2)3, 58-9°, 140-6°/0.05, 70; II,
     m-O2NC6H4, (CF2)3, 86°, -, 50; II, p-AcOC6H4, (CF2)3, 76-7°,
     160-5°/0.03, 65; II, m-EtO2CC6H4, (CF2)3, -, 149-52°/0.02,
     65; II, p-MeO2-CC6H4, (CF2)3, 130°, -, 55; I, 4,6-dimethoxy-2-s-
     triazinyl, (CF2)3H, 34-8°, 130°/0.2, 20; II,
     4,6-dimethoxy-2-s-triazinyl, (CF2)3, 115-18°, -, 1; II,
     3,4-(MeO2C)2C6H3, (CF2)3, -, -, 72; I, \alpha-naphthyl, HO2C(CF2)3, -, -,
     39; I, 2-methyl-1-naphthyl, n-C7F15, -, -, 45; I, m-AcOC6H4, n-C3F7, -,
     92-4°/18, 65; and II, 2-thienyl, (CF2)3, -, -, 30. Also prepared was
     m-Ph(CF2)3C6H4(CF2)3C6H4(CF2)3Ph-m.
ΙT
     18450-33-4P 21250-01-1P 21250-02-2P
     21250-03-3P 21250-06-6P 21301-84-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
RN
     18450-33-4 HCAPLUS
CN
     Benzene, 1,1'-(1,1,2,2,3,3-hexafluoro-1,3-propanediyl)bis[3-methyl- (9CI)
     (CA INDEX NAME)
```

RN 21250-01-1 HCAPLUS

CN Benzoic acid, 3,3'-(1,1,2,2,3,3-hexafluoro-1,3-propanediyl)bis-, diethyl ester (9CI) (CA INDEX NAME)

RN 21250-02-2 HCAPLUS

CN Benzoic acid, 3,3'-(hexafluorotrimethylene)di-, dimethyl ester (8CI) (CA INDEX NAME)

RN 21250-03-3 HCAPLUS

CN Benzoic acid, 4,4'-(1,1,2,2,3,3-hexafluoro-1,3-propanediyl)bis-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{MeO-C} & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 21250-06-6 HCAPLUS

CN 1,2-Benzenedicarboxylic acid, 4,4'-(1,1,2,2,3,3-hexafluoro-1,3-propanediyl)bis-, tetramethyl ester (9CI) (CA INDEX NAME)

RN 21301-84-8 HCAPLUS

CN Benzene, 1,1'-(1,1,2,2,3,3-hexafluoro-1,3-propanediyl)bis[3-(1,1,2,2,3,3-hexafluoro-3-phenylpropyl)- (9CI) (CA INDEX NAME)

$$(CF_2)_3$$
—Ph
 $(CF_2)_3$ —Ph
 $(CF_2)_3$ —Ph
 $(CF_2)_3$ —Ph

L125 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:618274 HCAPLUS

DN 135:195695

 ${\tt TI}$ Fluorous reaction and separation methods

IN Curran, Dennis P.; De Frutos Garcia, Oscar; Oderaotoshi, Yoji

PA University of Pittsburgh, USA

SO PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

FAN.CNI I			WIND DAME			A DOLL TO A MILONIA A MA												
	PATENT NO.			KIND DATE			APPLICATION NO.											
ΡI	WO	2001	 0613:	32		A1	_	2001	0823	1						2	0010	 216 <
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
			CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
			ΗU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,
			LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	ΝZ,	PL,	PT,	RO,	RU,
			SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	VN,	YU,
			ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM					
		RW:						MZ,										
								GB,									TR,	BF,
								GΑ,										
																-		<u>218 ≤</u>
		2400																216 <
	ΕP																	216 <
		R:						ES,	-			•	LI,	LU,	NL,	SE,	MC,	PT,
							•	RO,	•	•	•							
		2003																216 <
		2004										004-	8310	87		2	30404	123 <
PRAI		2000		_		Α		2000										
	WO	2001	-US5	065		W		2001	0216	< -	-							
GI																		

Me
$$\mathbb{R}^1$$
 \mathbb{N} \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^2 \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^2 \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^2 \mathbb{R}^4 \mathbb{R}^4

AB The present invention provides a fluorous-tagging strategy comprising the steps of: a. tagging a first organic compound with a first tagging moiety to result in a first tagged compound; b. tagging at least a second organic compound

with a second tagging moiety different from the first tagging moiety to result in a second tagged compound; and c. separating the first tagged compound from a mixture including the second tagged compound using a separation technique

based upon differences between the first tagging moiety and the second tagging moiety, in the synthesis and separation of mixts. of organic compds. including analogs of mappicine, such as, [I; R1 = H, aryl, SiMe2Bu-t; R2 = alkyl, CH2Ph; R3 = alkyl; R4 = alkyl, fluoroalkyl]. Thus, mappicine analogs, such as, I [R1 = H, Ph, SiMe2Bu-t; R2 = Et, Bu-t, CH2Ph; R3 = Me, (Me)2CH,; R4 = C6H13, C4F9, C6F13, C8F17, C10F21] were prepared via radical cyclization of N-alkylated pyridone [II; R1 = H, Ph, SiMe2Bu-t; R2 = Et, Bu-t, CH2Ph; R3 = Me, (Me)2CH,; R4 = C6H13, C4F9, C6F13, C8F17, C10F21] (also prepared) and 4-methylphenyl isonitrile and separated by preparative HPLC with a FluofixTM column.

IT 356055-76-0P 356055-77-1P 356055-78-2P 356055-79-3P 356055-83-9P 356055-85-1P 356055-86-2P 356055-87-3P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorous-tagging strategy for synthesis and separation of mixts. of organic compds.)

IT 356055-80-6P 356055-81-7P 356055-82-8P 356055-84-0P 356055-88-4P 356055-89-5P 356055-90-8P 356055-91-9P 356055-92-0P 356055-93-1P 356055-94-2P 356055-95-3P 356055-96-4P 356055-97-5P 356055-98-6P 356055-99-7P 356056-00-3P 356056-01-4P 356056-02-5P 356056-03-6P 356056-04-7P 356056-05-8P 356056-06-9P 356056-07-0P 356056-08-1P 356056-27-4P 356056-32-1P 356056-30-9P 356056-31-0P 356056-32-1P 356056-33-2P 356056-37-6P 356056-38-7P 356056-39-8P 356056-40-1P 356056-41-2P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(fluorous-tagging strategy for synthesis and separation of mixts. of organic compds.)

IT 356055-76-0P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorous-tagging strategy for synthesis and separation of mixts. of organic compds.)

RN 356055-76-0 HCAPLUS

CN Benzenemethanol, 4-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)- (9CI) (CA INDEX NAME)

$$CH_2-CH_2-(CF_2)_5-CF_3$$

 $HO-CH_2$

RETABLE

Referenced Author (RAU)		PG Referenced (RPG) (RWK)	File
Jackson	1994	US 5340453	A HCAPLUS
Wang	1984	US 4454233	

=> d his

L22

L23

L24

(FILE 'HOME' ENTERED AT 06:54:13 ON 12 APR 2005) SET COST OFF

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FILE 'HCAPLUS' ENTERED AT 06:55:09 ON 12 APR 2005
L1
               1 S US20040073054/PN OR (US2003-617431# OR WO2003-US21686 OR US20
                 E FLUOROUS/PA, CS
L2
              40 S E3-E16
                 E ZHANG W/AU
L3
            1582 S E3-E26
                 E ZHANG WEI/AU
            6827 S ZHANG WEI?/AU
L4
                 E LUO Z/AU
L5
              63 S E3,E19
                 E LUO ZHI/AU
L6
              69 S E3, E32, E86
                 E NAGASHIMA T/AU
L7
             168 S E3,E5
                 E TADAMICHI/AU
                 E CHEN C/AU
\Gamma8
           1553 S E3,E18,E22
                E CHEN CHRIS/AU
              7 S E3, E7
L9
L10
             29 S E15-E18
                E YU M/AU
L11
             207 S E3,E24
                 E YU MARVIN/AU
L12
             17 S E3-E5
                 E SUNGWHAN/AU
                 SEL RN L1
     FILE 'REGISTRY' ENTERED AT 06:59:31 ON 12 APR 2005
L13
             84 S E1-E84
L14
              1 S C22H14F17NO5 AND L13
L15
              1 S C18H11F17O2 AND L13
L16
              1 S C29H18F17NO5 AND L13
L17
              1 S C16H8BRF17 AND L13
L18
              2 S C17H10BRF17 AND C6/ES
L19
              0 S C27H14CLF17
L20
             39 S L13 AND F/ELS
L21
             35 S L20 NOT L14-L18
```

FILE 'HCAOLD' ENTERED AT 07:07:43 ON 12 APR 2005

24 S L21 AND F>=4

28 S L14-L17, L22

30 S L18, L23

```
L25
              2 $ L24
     FILE 'REGISTRY' ENTERED AT 07:08:18 ON 12 APR 2005
L26
             22 S L24 AND NR>=1
L27
              8 S L24 NOT L26
     FILE 'HCAPLUS' ENTERED AT 07:09:29 ON 12 APR 2005
L28
             19 S L26
L29
              5 S L28 AND L1-L12
L30
              4 S L29 AND (FLUOR? (L) TECH?) / PA, CS
L31
              5 S L29, L30
L32
             14 S L28 NOT L31
L33
             12 S L28 AND (PD<=20020711 OR PRD<=20020711 OR AD<=20020711)
L34
              3 S L32 NOT L33
     FILE 'REGISTRY' ENTERED AT 07:12:31 ON 12 APR 2005
     FILE 'HCAPLUS' ENTERED AT 07:12:40 ON 12 APR 2005
     FILE 'REGISTRY' ENTERED AT 07:13:23 ON 12 APR 2005
L35
                STR
                E F/ELS
L36
                SCR 1968
L37
             50 S L35 AND L36
L38
          35612 S L35 AND L36 FUL
                SAV TEMP L38 SHIAO617A/A
L39
                STR L35
L40
           50 S L39 SAM SUB=L38
L41
           7096 S L39 FUL SUB=L38
                SAV TEMP L41 SHIAO617A1/A
L42
                STR L39
L43
            50 S L42 SAM SUB=L41
L44
           4708 S L42 FUL SUB=L41
                SAV TEMP L44 SHIAO617A2/A
L45
                STR L42
L46
            50 S L45 SAM SUB=L44
           3542 S L45 FUL SUB=L44
L47
                SAV TEMP L47 SHIAO617A3/A
L48
           3179 S L47 NOT (PMS OR MXS)/CI
L49
             72 S L48 AND NC4/ES
L50
             6 S L49 AND (C18H14F9NO5 OR C20H14F13NO5 OR C23H14F19NO5 OR C22H1
L51
            29 S L48 AND OC4/ES
L52
            291 S L48 AND S/ELS NOT L49-L51
L53
            289 S L52 NOT (CCS/CI OR SQL/FA)
L54
                STR L35
L55
              1 S L54 SAM SUB=L48
L56
              7 S L54 SAM SUB=L38
L57
            130 S L54 FUL SUB=L38
                SAV L57 TEMP SHIAO617A4/A
L58
             23 S L57 AND L41
L59
              3 S L58 AND (C19H12CLF17O2 OR C18H8CLF17O2 OR C18H10CLF17O2)
L60
              9 S L50, L59
                SAV TEMP L60 SHIAO617A5/A
L61
              7 S L60 NOT L26
     FILE 'HCAOLD' ENTERED AT 07:55:25 ON 12 APR 2005
L62
              0 S L61
     FILE 'HCAPLUS' ENTERED AT 07:55:28 ON 12 APR 2005
L63
              6 S L61
L64
              1 S L63 AND L1-L12
L65
              4 S L63 AND (PD<=20020711 OR PRD<=20020711 OR AD<=20020711)
L66
              5 S L64, L65
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L67 1 S L63 NOT L66
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FILE 'REGISTRY' ENTERED AT 07:56:30 ON 12 APR 2005

FILE 'HCAPLUS' ENTERED AT 07:56:48 ON 12 APR 2005

FILE 'REGISTRY' ENTERED AT 07:57:42 ON 12 APR 2005 L68 STR

L69 50 S L68

L71

L70 2012368 S 46.150.18/RID AND F/ELS

50 S L68 AND L36 SAM SUB=L70

L72 SCR 1044

L73 50 S L68 AND L36 AND L72 SAM SUB=L70

L74 37805 S L68 AND L36 AND L72 FUL SUB=L70 SAV TEMP L74 SHIAO6A7B/A

L75 905 S L38 AND SI/ELS NOT (PMS OR CCS)/CI

L76 STR L39

L77 STR L76

L78 12 S L77 FUL SUB=L38

L79 3 S L78 AND 1/CL

L80 1 S L79 AND C32H18CLF39O2SI

FILE 'HCAPLUS' ENTERED AT 08:08:54 ON 12 APR 2005 L81 2 S L80

FILE 'REGISTRY' ENTERED AT 08:09:29 ON 12 APR 2005

SAV L78 SHIAO617A6/A DEL SHIAO6A7B/A

SAV TEMP L74 SHIAO617B/A

L82 STR L45

L83 50 S L82 SAM SUB=L74

L84 16196 S L82 FUL SUB=L74

SAV TEMP L84 SHIAO617B2/A

L85 STR L82

L86 50 S L85 SAM SUB=L84

L87 STR L85

L88 STR L82

L89 16283 S L88 FUL SUB=L74

DEL SHIAO617B2/A

SAV TEMP L89 SHIAO617B2/A

L90 50 S L87 SAM SUB=L89

L91 STR L87

L92 50 S L91 SAM SUB=L89

L93 7961 S L91 FUL SUB=L89

SAV TEMP L93 SHIAO617B3/A

. L94 STR L91

L95 50 S L94 SAM SUB=L89

L96 4820 S L94 FUL SUB=L89

SAV TEMP L96 SHIAO617B4/A

L97 11342 S L93,L96

L98 STR

L101

L99 50 S L98 SAM SUB=L97

L100 11327 S L98 FUL SUB=L97

FILE 'HCAPLUS' ENTERED AT 08:40:52 ON 12 APR 2005

2509 S L97

L102 4 S L1-L12 AND L101

SEL HIT RN

FILE 'REGISTRY' ENTERED AT 08:41:38 ON 12 APR 2005

L103 63 S E1-E63

L104 58 S L103 NOT L26, L61, L80

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FILE 'HCAPLUS' ENTERED AT 08:42:48 ON 12 APR 2005
L105
           2505 S L101 NOT L102
L106
           2228 S L105 AND (PD<=20020711 OR PRD<=20020711 OR AD<=20020711)
L107
            460 S L106 AND BENZEN?/SC,SX
L108
              0 S L107 AND TAGGING
L109
              0 S L107 AND TAG?
L110
              3 S L107 AND SCAVEN?
                E SCAVEN/CT
               E E19+ALL
L111
           6664 S E2+NT
                E HALOALKYLATION/CT
L112
            504 S E3-E12
                E E3+ALL
L113
            492 S E3+NT
                E COMBINATORIAL/CT
L114
          22605 S E7+OLD, NT, PFT, RT
L115
          37252 S E5+OLD, NT, PFT, RT
                E E5+ALL
          17055 S E6+OLD, NT, PFT, RT
L116
L117
            58 S L106 AND L111-L116
L118
             39 S L117 AND L107
L119
             48 S L117 AND L112, L113
L120
              0 S L119 AND L111
L121
              0 S L119 AND L114-L116
L122
             19 S L117-L119 AND P/DT
L123
             15 S L122 AND L112,L113
     FILE 'REGISTRY' ENTERED AT 08:47:53 ON 12 APR 2005
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FILE 'HCAPLUS' ENTERED AT 08:48:07 ON 12 APR 2005

L124 4 S L122 NOT L123, L102

L125 1 S L124 AND FLUOROUS REACTION/TI

=>